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3-Dimensional alignment of micro components
using liquid droplets

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*To my parents George and Jacqueline, and my girlfriend Amanda Chang,
whose love and support helped me complete this work*

ABSTRACT

This thesis presents an improved understanding of how liquid surface tension controls component alignment with a focus on factors associated with fabrication quality; offering insight into the impact of adopting the novel additive manufacturing route, and to provide means for designers and engineers, who are not intimately familiar with the dynamics of liquid alignment, to incorporate such features into their work. The work is supported by several novel models and methods created during the PhD project.

The research objectives were addressed through a combination of experimental work, which established the feasibility of utilising additively manufactured binding sites for liquid droplet alignment tasks, and modelling using Surface Evolver, which simulated component alignment tasks and the effect of imperfect binding site geometry.

Droplet shape on circular and square binding sites with varying edge geometry was investigated and significant increases in contact angle of liquid water droplets were observed compared to the plain substrate, with clear benefits observed for structures with actual edge geometries $<90^\circ$ which achieved repeatable alignment with a mean final component misalignment of 31 μm and 14 μm standard deviation.

Simulations showed that as edge radius of the binding site increased the ability to stop droplet motion around the edge diminished. For binding site undercut angles $<90^\circ$ an energy penalty was observed which provided a barrier to droplet motion down the sidewall. For binding site angles $>90^\circ$ an energy benefit was observed which encouraged droplet motion down the sidewall.

The integration of Surface Evolver generated data into a commercial CAE package for the purpose of an optimisation design study was presented which highlighted the potential of the technique for analysing complex geometries which would otherwise be extremely difficult in Surface Evolver.

LIST OF PUBLICATIONS AND PRESENTATIONS

J. K. Overton, P. K. Kinnell, S.D.A. Lawes, S. Ratchev (2015) *High precision self-alignment using liquid surface tension for additively manufactured micro components*. In: Precision Engineering Journal, Volume 40, April 2015, 230-240.

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LIST OF ABBREVIATIONS

1D (2D, 3D)	One Dimensional (Two Dimensional, Three Dimensional)
2PP	Two-Photon Polymerisation
CAD	Computer Aided Design
CAE	Computer Aided Engineering
CFD	Computational Fluid Dynamics
CGS	Centimetre, Gram, Second
DMD	Digital Micromirror Device
DOF	Degrees of Freedom
ECM	Electrochemical Machining
EDM	Electro Discharge Machining
EMM	Electrochemical Micro Machining
FDM	Fused Deposition Modelling
FE	Finite Element
GUI	Graphical User Interface
HPC	High Performance Computer
IEG	Inter-electrode Gap
IH	Integrated Hardened
LB-ADSA	Low Bond – Axisymmetric Drop Shape Analysis
LBM	Laser Beam Machining

LBMM	Laser Beam Micro Machining
LCD	Liquid Crystal Display
LIGA	Lithographie, Galvanoformung, Abformung (Lithography, Electroplating and Moulding)
MBD	Multibody Dynamics
MKS	Metre, Kilogram, Second
NI	National Instruments
PMMA	Poly(methyl methacrylate)
PMSL	Projection-Micro-Stereolithography
PVC	Polyvinyl Chloride
RIE	Reactive Ion Etching
SE	Surface Evolver
SE-FIT	Surface Evolver – Fluid Interface Tool
SEM	Scanning Electron Microscope
SLS	Selective Laser Sintering
SMA	Shape Memory Alloy
STL	Standard Triangulation Language
TCL	Triple Contact Line
UV	Ultraviolet
WUXGA	Widescreen Ultra Extended Graphics Array

LIST OF SYMBOLS

Symbol	Description	Units
B_o	Bond number	-
E_o	Eötvös number	-
F	Force	N
g	Acceleration due to gravity	$m\ s^{-2}$
γ	Surface tension	N/m
ρ	Density	$Kg\ m^{-3}$
m	Mass	Kg
θ	Contact angle	Degrees or Radians
S	Interfacial area	m^2
λ_c	Capillary length	m
ε_{vdw}	Interaction energy between two molecules for van der Waals force	J

Chapter 1

1 INTRODUCTION

1.1 Problem definition and motivation

Industrially manufactured products are typically assemblies made up of many separate and often dissimilar components. The assembly techniques required to realise these finished items are therefore of key importance to product generation. The micro component industry is rapidly growing and the continual trend of component miniaturisation has led to its own set of challenges that are not present in the macro domain. Simple pick-and-place operations become complex issues due to scaling effects, as parts become smaller gravity is no longer the dominant force. This is because surface forces scale with length, whereas gravity scales with length cubed [1]. This results in release problems due to adhesion forces between components and micro handling tools. Surface-related forces such as van der Waals, electrostatic and surface tension dominate over gravitational force, which have led to novel handling strategies becoming the focus of much work. This includes the development of techniques such as micro grippers [2-4], vacuum grippers [5], freeze grippers [6], as well as those based on electrostatic forces [7, 8].

An additional challenge for micro assembly in an industrial environment is that the process must be both fast and precise. Current methods make use of robotics to manipulate and place components; however these solutions either build assemblies with sub-micron accuracy at low speeds, or at high assembly speeds but with low accuracy [9]. There is also a cost trade-off to be made with faster more accurate systems being significantly more expensive. To lessen the challenge of micro assembly an interesting concept is that of component self-assembly. Liquid self-assembly of components is an attractive alternative to traditional robotic pick-and-place techniques as it can offer very high final positional accuracy with fairly coarse initial placement. This means lower cost, faster pick-and-place systems, or the replacement of robotic pick and place with manual pick-and-place; leading to the advantages of either increased system flexibility, or reduced cost and higher throughput. The underlying

concept behind liquid self-assembly is that features produced on the components can control droplet shape, and therefore surface tension, in such a way that the lowest energy state for the liquid is achieved when the components are well aligned. These features are typically referred to as either binding sites, or receptor sites. Throughout this thesis the former reference will be used. The principle of liquid self-assembly is illustrated in Figure 1-1 which shows the droplet in place prior to assembly (a); followed by the drop wetting to both the static surface and the part (b). At this stage the non-symmetrical nature of the liquid surface results in surface tension forces that tend to move the part to a state of lowest surface energy; once the lowest surface energy state has been reached all surface tension forces are balanced (c).

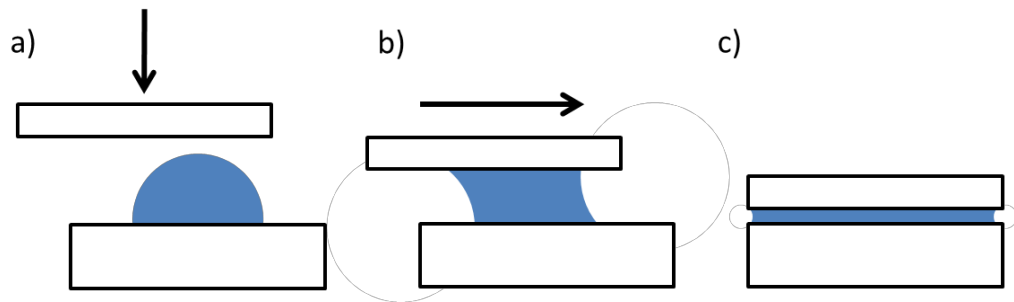


Figure 1-1: Self-alignment of component using liquid surface tension. a) Liquid droplet dispensed onto binding site and component moved into place, b) component comes into contact with liquid droplet and meniscus is formed, c) restoring forces act on component and it aligns to shape of binding site due to energy minimisation.

Improvements in additive manufacturing processes have seen them move from a purely prototyping technique, to one that is increasingly being used for final product generation. This has led to high levels of design and production flexibility for micro components. With this flexibility, increased demands are being placed on microhandling tools and assembly techniques which must be able to assemble these components into finished products while adapting to highly customisable, small batch components. Liquid self-assembly offers a promising solution to these challenges as additive manufacturing allows the freedom to incorporate binding sites for alignment directly into the component without the need for additional process steps, and at no additional cost.

1.2 Aim and objectives

The aim of this work is to **develop an improved understanding of how liquid surface tension controls component alignment with a focus on factors associated with fabrication quality; offering insight into the impact of adopting the novel additive manufacturing route, and to provide means for designers and engineers, who are not intimately familiar with the dynamics of liquid alignment, to incorporate such features into their work.** This is needed to provide cost-effective and accurate assembly procedures that can be applied to the growing MEMS and micro component industries.

A number of key requirements must be fulfilled in order to understand the self-assembly process in terms of binding site design, component design and the interaction during the assembly process. To realise the project aim a number of methods and models need to be established to capture and predict the effects of various design decisions on the assembly process. This leads to the formation of the following objectives:

- Characterise a suitable additive manufacturing process for the production of liquid alignment binding sites;
- Investigate the effect of binding site edge geometry on the ability to control liquid spreading, and its role as an early indication of assembly reliability;
- Define a model to examine the effect of binding site edge geometry on the liquid droplet during assembly;
- Define a series of models expressing the forces generated by a liquid droplet under typical self-assembly conditions and how this can be applied in a design context;
- Demonstrate the application of the above models and insights in the design of components for a micro component alignment test case.

The completion of the first two objectives provide an understanding of the optimum edge geometry required to control the spreading of liquid droplets

needed for self-assembly processes. This leads to the creation of the models which investigate specific factors of the binding site design and the role these play on alignment capability. The fourth objective models a typical self-assembly process and analyses the forces generated by liquid droplet during the alignment process. The final objective moves the focus to the amalgamation of the previously created methodologies and models to a micro component test case. A more detailed explanation of the objectives and how they contribute to the overall design methodology is presented in chapter 3, section 3.1.

1.3 Thesis structure

A summary of the nine individual chapters found in the thesis is presented below, summarised as a graphical representation in Figure 1-2.

Chapter 1 presents the research problem, the motivation behind this work and the project aim and objectives.

Chapter 2 provides a review of the current literature. An introduction to micro components is presented followed by the current assembly and handling strategies utilised to manipulate these components and their associated challenges. The reader is then given a brief overview of microfluidics with a specific focus on self-assembly techniques, before proceeding to a discussion of the physics prevalent in the domain. The chapter then presents techniques for computational analysis of microfluidics and computer aided engineering tasks, which are expanded upon in chapters 6, 7 and 8. The chapter is concluded by identifying the project related knowledge gaps that will be addressed by this thesis.

Chapter 3 introduces the research methodology and details how the project objectives will be met and linked to the overall aim of the work. The assumptions and limitations applied to the work are explained, as well as the experimental techniques and fabrication processes used in the following core research chapters.

Chapter 4 presents the design rationale used to produce components intended for self-assembly applications using liquid surface tension. The manufacturing was carried out using an EnvisionTec Perfactory which is a projection micro stereolithography (PMSL) technique of additive manufacturing. The chapter addresses the various methods developed in order to reliably and accurately produce structures which can be used in the alignment of micro components using liquid surface tension.

Chapter 5 presents a broad experimental investigation of additively manufactured binding sites. Cross sectional analysis of the structures is performed to assess the quality of the manufactured components. The concept is then applied to the assembly of flat chip-like structures under three challenging assembly conditions. These observations highlight specific challenges which are investigated in chapter 6 by means of a numerical modelling approach.

Chapter 6 presents numerical modelling of microdroplet alignment using the Surface Evolver software. Spring constants are determined for discrete component misalignments for the six degrees of freedom of the component which are compared to simple analytical solutions.

Chapter 7 presents numerical modelling using Surface Evolver of the effect of imperfect geometric features introduced during manufacturing, such as rounded edges and undercut edge geometry of binding sites, and how these influence the surface energy of the system.

Chapter 8 considers the design challenge of incorporating liquid alignment features for a practical test case. The example considers micro components with high aspect ratio, and shows the capabilities of such an approach for complex and highly 3-dimensional systems. A numerical model is created using Surface Evolver and the generated data is then incorporated into a commercially available CAE package in order to perform a design optimisation. The results are validated against an analytical solution and experimental investigation.

Chapter 9 summarises the key findings and results from the project and suggests areas of interest to be addressed in future work.

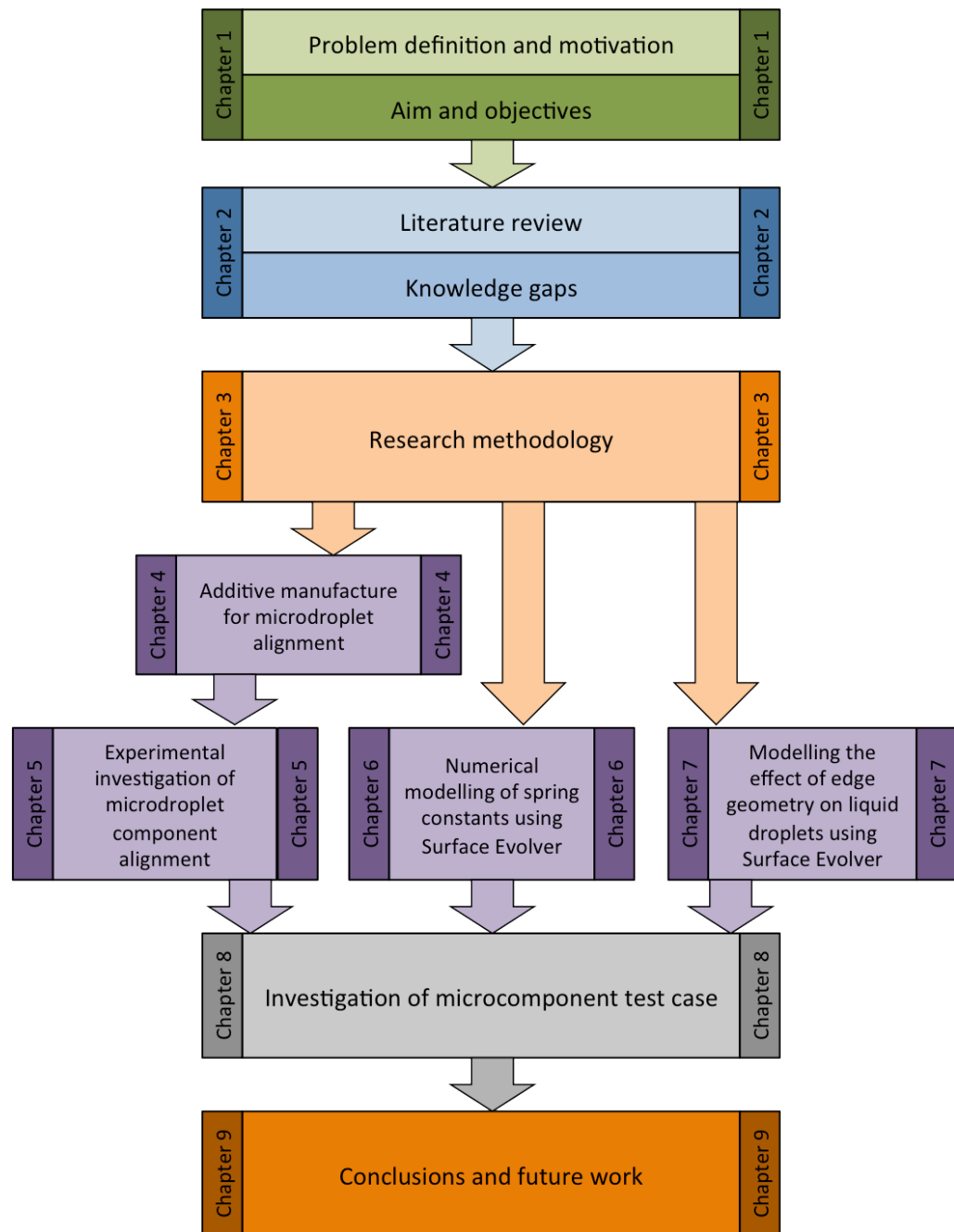


Figure 1-2: Structure of the presented thesis.

Chapter 2

2 LITERATURE REVIEW

This chapter is intended to provide the reader with an overview of the micro components, and microfluidics domains and to outline the importance of the self-assembly procedure to industrial manufacturing applications. The chapter begins with an introduction to micro components and defines the scale that is addressed in the thesis. The current assembly and handling strategies for micro components are then outlined. This is followed by an explanation of microfluidics and an examination of the physics governing micro droplet assembly. The chapter then presents the computational tools available for microfluidic analysis. The chapter is concluded with a summary and identification of the knowledge gaps that need to be addressed in order to achieve the project aim.

2.1 Micro components

The drive for miniaturisation of components in order to achieve more functionality, in less space, and at a lower cost over the last few decades has led to the emergence of the micro components industry. Although the term “micro components” is widely used, this does not necessarily denote that the product size is of a few microns. Indeed Alting et. al presented the following definition: “Micro engineering deals with development and manufacture of products, whose functional features or at least one dimension are in the order of μm . The products are usually characterized by a high degree of integration of functionalities and components” [10]. Figure 2-1 illustrates that for a micro part the component, feature size and accuracy can all be of the same magnitude. As a comparison, in the macro domain, the product will typically fit in a box of dimensions 200 x 200 x 200 mm, with feature sizes in the mm to cm range, assembled with positional accuracies as small as 10 μm [11].

The work presented in this thesis is concerned with components whose dimensions fall within the range of 0.4 – 12.5 mm, with features in the micron

range. These components are small enough for gravitational forces to begin to become negligible, yet are still able to be seen with the naked eye.

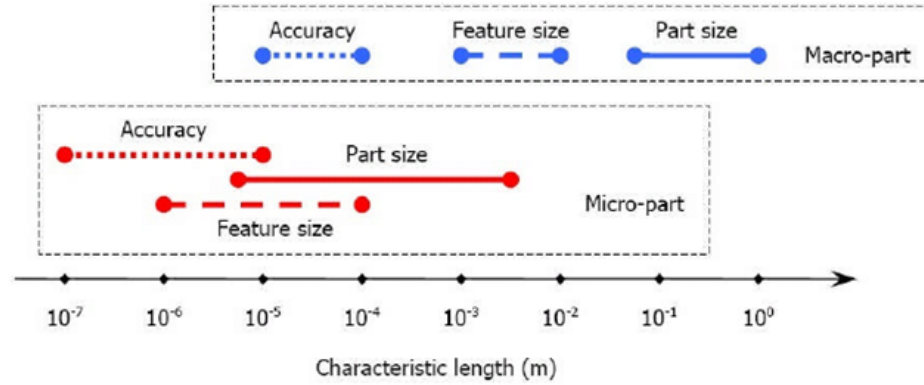


Figure 2-1: Scale of macro vs. micro engineering [11].

Micro components are used for a diverse range of applications in a number of industries including automotive, aerospace, telecommunications, optics, and biomedical. They are produced from a range of materials and manufacturing methods.

Industrial products typically consist of multiple components, each designed to perform specific functions. These are likely to be made of dissimilar materials and geometries which must be handled, assembled, and sometimes joined, in order to realise the final product. The assembly task is therefore of key importance to product generation and will be the topic of the following section.

2.2 Micro assembly and handling

One of the major challenges arising from micro assembly tasks is the handling of components. It is relatively easy to pick up an object, however the accurate placement and release is much more difficult due to adhesive forces. The task is not as straightforward as simply reversing the pick-up operation [12]. This means that methods which were developed for macro component handling which primarily rely on mechanical grip force to pick up, and the component weight to release cannot be directly applied to micro assembly tasks [13]. This

has led to the development of novel handling strategies which aim to overcome these scaling effects and will be the subject of this section of the literature review.

2.2.1 *Current methods*

Due to the scaling effects whereby surface forces dominate over gravitational, new handling strategies have had to be developed in order to address emerging micro assembly tasks. Robotic arms are often necessary to achieve the assembly task and the point at which this interacts with the environment is known as the end effector. These can include; mechanical grippers, capillary grippers, freeze grippers, electrostatic grippers and vacuum grippers. Other manipulation methods include laser trapping, and acoustical levitation. Each of these will now be described to familiarise the reader with the subject. A diagram of a typical assembly process is shown in Figure 2-2.

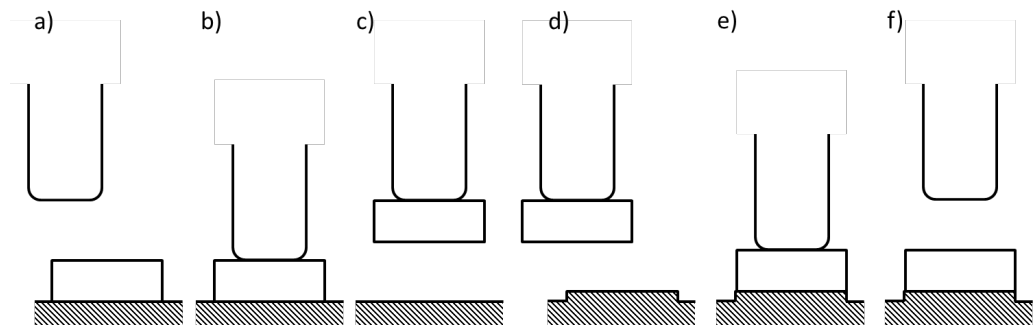


Figure 2-2: Diagram illustrating a typical assembly process. a) Gripper approaches component, b) gripper makes contact with component, c) component is picked up, d) component is moved towards target location, e) component is placed on target location, f) component released and gripper moves away.

Mechanical grippers are the most widespread gripper in industry and make use of miniaturised tweezers to pick up the component. The most common method of actuating the tweezers is through the use of smart materials, with the most prevalent being piezoelectric [2, 14-17]. Other actuation methods include pneumatic [18, 19], shape memory alloy (SMA) [20], electrothermal [21, 22], and electrostatic [23, 24]. The main aspect that needs to be considered with mechanical gripper design is not so much whether the force is sufficient to pick

up the component, but rather that the clamping force does not cause damage [25].

Capillary grippers rely on the capillary forces of a liquid droplet between the gripper and the component. The liquid droplet wets to both surfaces forming a liquid bridge (meniscus) which enables the part to be manipulated [26-30] (Figure 2-3). The gripping process is affected by a number of factors including the properties of the liquid, environment in which the operation is taking place, and the surface properties of both the component and gripper [29]. This method is not suitable for porous materials, or ones with hydrophobic surfaces. A detailed explanation of the physics involved in liquid droplet alignment is introduced later in the literature review in section 2.4.

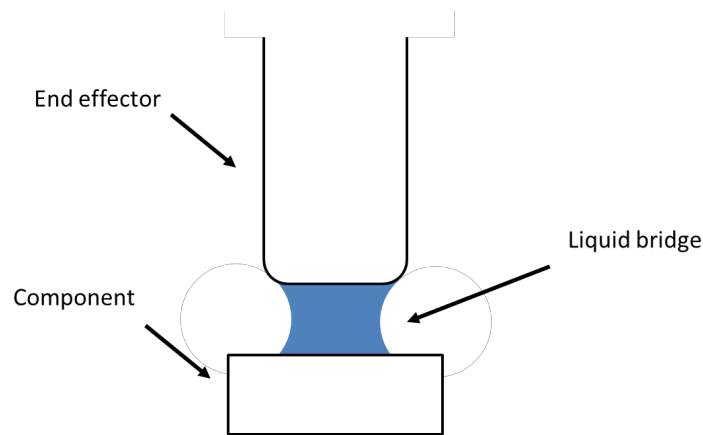


Figure 2-3: Diagram illustrating the operation of a capillary gripper.

Freeze grippers, also known as ice, or cryogenic grippers work under the same principle as the aforementioned capillary gripper, however after the liquid bridge is formed the liquid is frozen [31-33]. To release the component the end effector is simply heated to cause the interface to return to its liquid state. This offers certain advantages over other grippers as it provides high adhesion force without risk of damaging the component, and is much less affected by environmental and material surface properties. It is also capable of offering fast cycle times and high reliability [34].

Electrostatic grippers rely on the attractive or repulsive force created between two particles with a charge difference in order to perform the handling operation (Figure 2-4). The charge difference is created by applying a voltage to the gripper which can be varied to alter the force. One of the challenges to this method is that residual charge left on the component can disturb further handling operations. There is also the risk of damaging electrically sensitive components. Component release is normally achieved by alternating the voltage potential of the gripper or by applying voltage potential to the target substrate [8, 35-37].

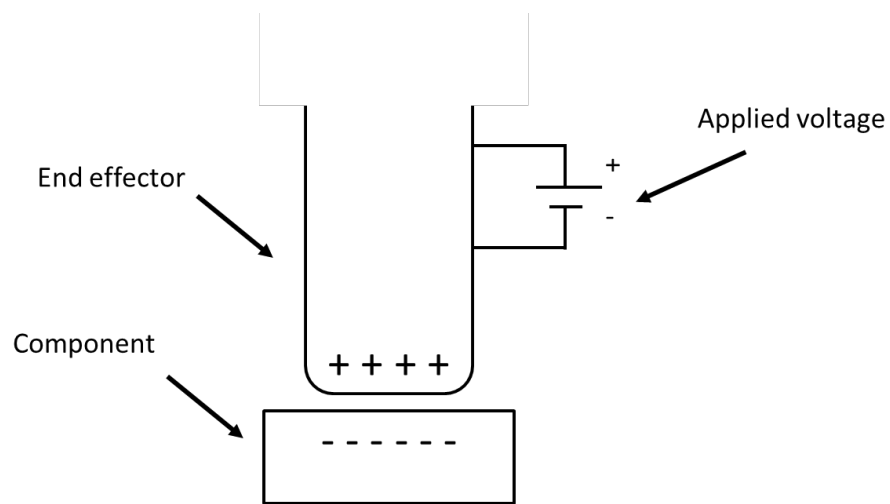


Figure 2-4: Diagram illustrating the principle of an electrostatic gripper.

Vacuum grippers (also known as suction grippers) typically consist of a glass pipette attached to a vacuum pump (Figure 2-5). The principle relies on the vacuum force to pick up the component, and simply switching off the pump, or reversing the air flow in order to achieve component release [5, 38-40]. As the principle relies on the pressure difference between the pipette and ambient atmosphere, the process cannot be used in a vacuum environment. It is also therefore unsuitable for porous materials.

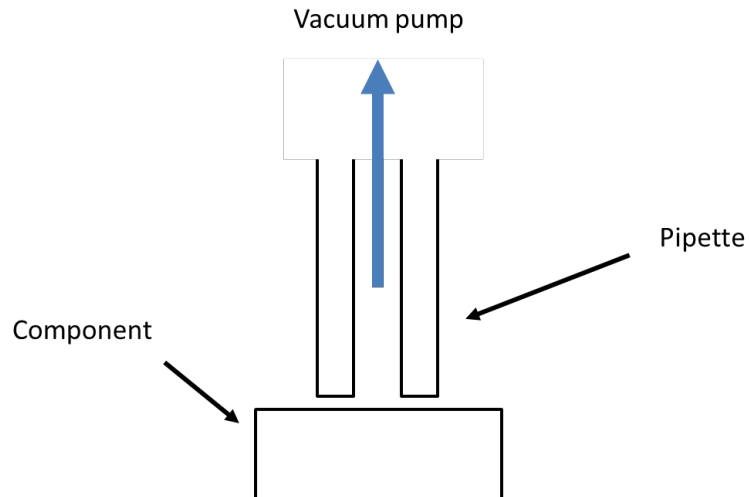


Figure 2-5: Diagram illustrating the principle of a vacuum gripper.

Magnetic grippers work on the principal that a force interaction is applied between the component and gripper through the motion of electrically charged particles. Magnetic grippers can be separated into two classifications: Electromagnets, where the motion occurs through electron movement from an applied current; or permanent magnets, where motion occurs from orbital electron movement. Although this technique is widely used in the macro domain, there are a number of limitations which make it less suitable when applied to micro components. Firstly, the scaling factor is to the third or fourth power of the characteristic length, resulting in the gripping force decreasing more rapidly than gravity as component dimensions decrease [41]. Additionally, the range of materials which can be manipulated is limited to ferromagnetic materials.

Laser trapping (also known as optical pressure gripping, or optical trap) uses the optical pressure of a light source to manipulate components. Due to beam reflection and refraction the component is subjected to an axial force which pushes it in the direction of the beam. There is also a radial gradient force which holds the component in the centre of the beam [42-45]. It is preferential for the method to be carried out in a liquid environment as it can help to damp component oscillations during handling [44]. The technique is particularly useful for handling very fragile and surface sensitive components as it is a non-

contact operation, however the grip force is very small, hardly reaching 1 nN [46].

Acoustical levitation uses acoustic waves to apply forces on a component. There are two methods: standing wave levitation, and near-field levitation. In standing wave levitation components can be held in the pressure nodes of an acoustical standing wave between a vibrating plate and a reflector (Figure 2-6). The static pressure distribution of the standing wave causes high frequency flow around the component. This results in a pressure differential which acts to centre the component in the wave (Bernoulli effect) [47-49]. Components of a few grams can be manipulated under atmospheric conditions, however the range can be extended if the procedure is performed in a micro gravity, or liquid environment [50]. Near-field levitation (also known as squeeze film levitation) replaces the reflector from the standing wave method with the levitated component. This means that if the separation distance can be kept small enough, components of any weight can be levitated [51-53]. One of the disadvantages of acoustical levitation is that the asymmetry in the flow field results in uncontrollable rotation of the component [54].

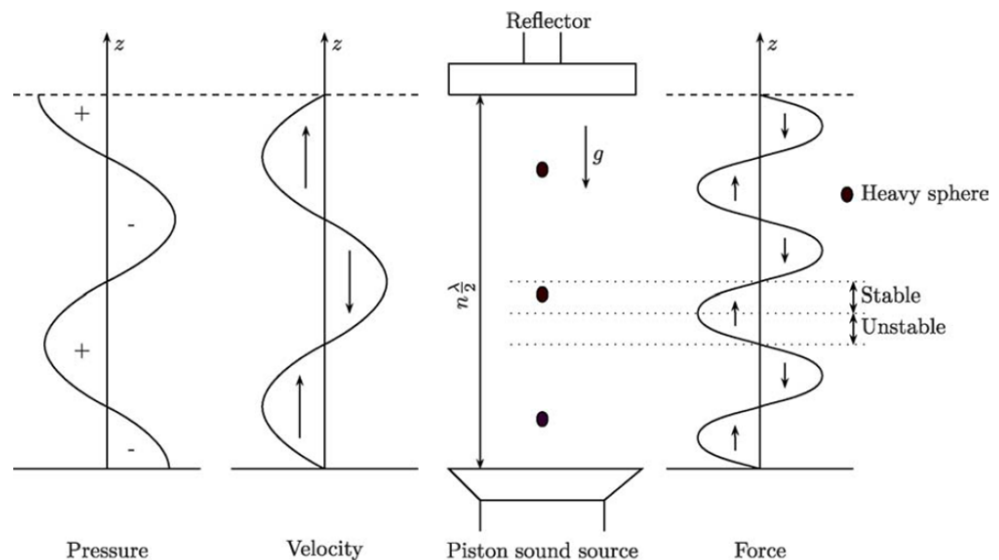


Figure 2-6: Levitation of dense spheres in an acoustic standing wave [54].

Having introduced the reader to the various micro manipulation techniques the section now moves onto the challenges faced during micro assembly operations, particularly the issue of component release from the end effector.

2.2.2 *Challenges at state of the art*

One of the major challenges for micro component assembly isn't whether the method can provide sufficient force to achieve pick up, but rather how the component is released. As mentioned previously, due to scaling laws gravity is no longer the dominant force acting on a component. This means that traditional assembly methods from the macro domain which would rely on the component mass to achieve release from the end effector are no longer applicable. For the non-contact techniques mentioned above (optical and acoustical) this problem does not apply, however for the other methods which contact the component additional attention must be given to the release stage.

Changing contact area between the end effector and component can be employed to reduce adhesion forces and initiate release [55]. In the case of capillary gripping this can be done by using a membrane that can be actuated to alter the liquid bridge during component release [27, 29]. An auxiliary tool can be used which has a lower contact area than the principle gripper, allowing the component to be released. Another technique is to laterally move the part against a structure to break the contact with the end effector. Permanent or temporary adhesion of the component can be employed to hold it in place before retracting the gripper. The use of acceleration or vibration have also been utilised to aid component release [56, 57].

An additional consideration is that some of the physical effects utilised by one grip principle can be detrimental to another. Capillary grippers rely on the formation of a liquid bridge between component and end effector, however for other techniques this is undesirable as it prevents component release. When there is moisture in the air condensation will always occur around surface contact points such as cracks and pores [58]. This can be overcome by controlling the humidity of the assembly environment [59], or by adding a

micro heater to the end effector [60]. As previously mentioned electrostatic charge is often seen as a disturbing factor in micro handling operations. It can be avoided by using conductive materials; however this may not be an option. There is the additional challenge of the build-up of an oxide layer over time which acts as an insulator. Over several days up to 1 nm of native oxide can build up on silicon in air at room temperature which can withstand a field charge of up 30 MV/cm [13, 61].

2.3 Microfluidics

Microfluidics is a multidisciplinary field that deals with the design, manufacture and formulation of devices that make use of volumes of fluids in the nanolitre (nL) or picolitre (pL) range. The devices themselves typically have dimensions in the millimetre (mm) to micrometre (μm) range. Microfluidic devices are used for a wide range of applications with the most well-known being the inkjet printer head. Other microfluidic devices include microvalves, micropumps, and lab-on-chip technology.

Microfluidics can be separated into two broad fields: continuous-flow, and droplet-based. Continuous flow microfluidics is based on the continual flow of fluid through micro channels. The flow of this fluid can be controlled by external pumps, integrated micropumps, microvalves, or micromixers. The development of integrated micropumps and microvalves has been driven by the needs of biological fluid handling for applications such as lab-on-chip and micro total analysis systems [62]. Additionally the thermal management of electronic devices in MEMS products using liquid flow is also being considered [63, 64].

The second area is that of droplet-based microfluidics which deals with discrete liquid volumes characterised by low Reynolds number and laminar flow.

Microfluidic devices have many attractive benefits including reduced overall size, reduced material costs, higher efficiency, and reduced sample and reagent

volumes (in the case of biological handling). Also due to their size they are well suited for parallel operations [65].

The work in this thesis is concerned with the area of droplet-based microfluidics, and in particular its application as a self-assembly technique for the assembly of micro components.

2.3.1 *Self-assembly*

Self-assembly can be seen as the spontaneous arrangement of pre-existing components into a defined orientation, without the need for additional input or manipulation. The parts must be able to move with respect to each other, and will be in a steady-state position when the attractive and repulsive forces are balanced [66]. For an excellent overview of the state-of-the-art in surface tension powered self-assembly the reader is referred to the seminal work by Syms et. al [67].

As was introduced in section 1.1, the concept behind liquid self-assembly is that features produced on a component can be utilised to control droplet shape, and therefore surface tension, in such a way that the lowest energy state for the liquid is achieved when the components are well aligned. The controlled spreading of the assembly liquid is a key factor in this process, and much work has been carried out into this area. Several approaches have been developed in order to alter the wetting properties of specific regions of a surface. These include (super)hydrophilic and (super)hydrophobic target sites [26, 68-72], (super)oleophilic and (super)oleophobic for oil-based liquids [73-75], micropillar arrays to create hydrophobic regions [76, 77], as well as most recently, receptor sites with sharp edges to inhibit liquid spreading [78-81]. These methods can be divided into two distinct areas; those which rely on altering the surface properties of specific regions to influence wetting behaviour, and those that utilise physical geometric structures to constrain liquid spreading. Until now the majority of the literature in this field focuses on applications involving the use of microchips assembled on silicon wafers [82-85], with modifications to surface properties being introduced through a post-

build process of coating, masking and etching. Typically this is achieved by thermally growing a silicon oxide layer on the wafer before a standard photolithography and reactive-ion etching (RIE) process is carried out to pattern the oxide layer [71, 78, 86] resulting in a hydrophilic surface. Other techniques [83, 84] also used black silicon coated with a fluoropolymer to realise a hydrophobic background material surrounding the binding sites.

Liquid self-assembly can also be utilised for parallel assembly tasks where multiple components are simultaneously assembled onto an array of binding sites. The technique is also referred to as multibatch self-assembly. Different methods have been implemented including using a multi-part tool to transfer multiple components [71], direct wafer-to-wafer transfer [87, 88], or using a stochastic technique where jumbled identical parts are placed in a liquid solution and agitated [82, 89-91].

Another well-established use of liquid self-assembly is that of deterministic folding of structures. In this method a liquid droplet of molten solder or glass is used to drive out of plane folding of an initially 2D net structure about a hinged joint, into a final 3D component [92-96]. The assembly begins as a 2D geometry with a meltable strip of solder or glass attached to the substrate and the hinged component. The assembly is then heated and the strip returns to its liquid state, causing the surface tension forces to impart a torque on the component. As the liquid moves towards its minimum energy state the component rotates about the hinged joint and out of plane. When the liquid has reached its minimum energy state the component is fully assembled and the liquid is allowed to cool and re-solidify (Figure 2-7).

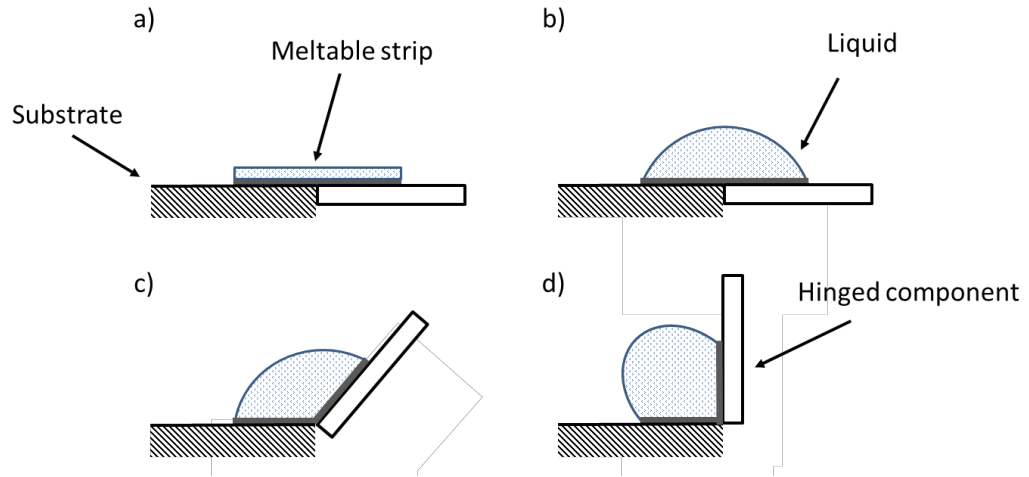


Figure 2-7: Diagram illustrating the process of out of plane folding of a hinged component. a) melttable strip attached to substrate and component, b) strip is heated, c) component folds out of plane about hinged joint due to surface tension, d) fully assembled component.

The final position of the component can be controlled by mechanical locking mechanisms which act to stop the angular rotation of the component at a fixed position [93, 97], or by careful control of the liquid volume [98]. The technique has successfully been used to assemble microoptoelectromechanical systems (MOEMS) such as micromirrors and scanners [67].

2.4 The physics of liquid droplet micro assembly

The physics acting on a component differ greatly when moving from the macro to the micro domain. Gravitational forces which dominate the macro domain become less significant as component dimensions decrease, while those that may have had a previously negligible effect begin to become the dominant force governing the system.

This section of the literature review introduces the reader to the overriding forces which play a role in the micro domain. It then moves onto forces specifically related to micro droplets and their interaction with the surrounding environment.

2.4.1 *Physical parameters*

To understand the effect of the various forces relative to each other it can be useful to compare them in terms of their geometrical dependency relative to length “L”. This means that surface scales with the second power of L (L^2), and volume the third power of L (L^3). It is assumed that the physical properties of the system are uniform and constant and density, viscosity, thermal conductivity etc. are not scaled with the geometry. The forces considered are van der Waals force, electrostatic force, and surface tension.

2.4.2 *Van der Waals force*

Van der Waals force is named after Dutch scientist Joahnnes Diderik van der Waals, who first proposed the idea to account for certain properties of non-ideal gases and liquids. It is the sum of the attractive and repulsive forces between molecules, which comprise London forces (force arising from shifts in electron cloud distribution), Keesom forces (force between two permanent dipoles), and Debye forces (force between a permanent dipole and a corresponding induced dipole) [99]. Of these three, the London forces are considered to be the most significant force. The interaction energy ϵ_{vdw} between two molecules can be expressed as:

$$\epsilon_{vdw} = -\frac{C}{r^6} \quad (2-1)$$

Where, C is a material and temperature dependent interaction constant, and r (m) is the distance between centres of two molecules.

It can be seen that the potential energy is highly dependent on the distance between molecule centres as it is inversely proportional to the sixth power of r. At the molecular scale the van der Waals force dominates and is responsible for the bonding of atoms and molecules, however as length increases this force quickly becomes negligible compared to gravity and surface tension forces.

The aforementioned microscopic approach neglects many-body interactions and retardation and a more rigorous approach proposed by Lifshitz is used when dealing with macroscopic bodies [100].

$$F = \frac{-Q^2}{(4\pi\epsilon_0\epsilon_3)(2D)^2} \left(\frac{\epsilon_2 - \epsilon_3}{\epsilon_2 + \epsilon_3} \right) \quad (2-2)$$

Where, Q (C) is the charge in a medium of dielectric constant ϵ_3 , D (m) is the distance between a plane surface of dielectric constant ϵ_2 , and ϵ_0 is the dielectric constant of vacuum.

2.4.3 *Electrostatic force*

Electrostatic force is the exchange of charge between two surfaces induced by an electrical field. Coulomb's Law which was developed by French physicist Charles Augustin de Coulomb states that the electrostatic force between two particles can be defined as [101]:

$$F = \frac{1}{4\pi\epsilon_0} \frac{qq'}{r^2} = K \frac{qq'}{r^2} \quad (2-3)$$

Where ϵ_0 is vacuum permittivity ($\approx 8.854 \times 10^{-12}$ F/m), q and q' is the magnitude between two point charges, separated by distance r (m).

When thinking about micro components the many particles that make up the component need to be considered. There the electrostatic force between two parallel plates can be defined as:

$$F = \frac{A\epsilon_0}{2d^2} (\Delta V)^2 \quad (2-4)$$

Where, A is the surface area perpendicular to the force, d (m) is the separation distance between the two plates, and ΔV is the applied voltage.

Electrostatic force typically occurs as a disturbing force in micro component handling, either through charge transfer, or through the build-up of charge in an insulating material. Equation (2-4) shows that for a given voltage the electrostatic force can be controlled by altering either the surface area, or the separation distance. As component dimensions are likely function driven, there may not be potential to alter the surface area. It can also be seen that the force scales with the inverse square of the separation distance and therefore has a much greater effect than surface area. This means that careful control of the separation distance can be utilised to either promote [102, 103], or reduce [55, 60, 104] the contribution of electrostatic forces.

2.4.4 *Surface tension*

At the interface between a liquid and a gas, the molecules in the bulk volume of the liquid are in contact with more neighbouring molecules than at the liquid surface. Although the molecules at the surface are in contact with gas molecules, these interactions are less frequent and offer less attraction than the liquid-liquid interactions of the bulk volume. This difference in interactions creates excess energy at the interface and is known as the surface energy [105]. When dealing with liquid-gas interfaces this energy is known as surface tension. Molecules at the surface will always look for other molecules to minimise this excess energy and move to a lower energy state, which results in a minimum energy surface. For a fixed liquid volume under no other forces, the shape adopted is that of a sphere. The symbol γ is used to denote surface tension, and it is given the units of force/area, typically in the form of SI unit N/m, or CGS (centimetre, gram, second) unit dyne/cm. The value of surface tension for a range of liquids in contact with air at 20°C is summarised in Table 2-1. The same principle is applied to an interface between a liquid and a solid, with liquid molecules at the interface attracted to the solid surface by van der Waals forces. When the attractions are strong the solid surface is said to be wetting, or hydrophilic, and displays a negative surface energy. When the attractions are weak the solid surface is said to be non-wetting, or hydrophobic, and the surface energy is positive [9]. When dealing with liquid-solid interfaces, the surface energy is normally referred to as interfacial energy. In

order to clarify which interface is being referred to the surface tension is normally given a subscript e.g. γ_{LG} would denote the surface tension at the liquid-gas interface.

The total energy of a surface E can be defined as:

$$E = \gamma S \quad (2-5)$$

Where, γ is the surface tension, and S is the interfacial area.

Liquid	Surface tension, mN/m	Liquid	Surface tension, mN/m
Acetic acid	27.6	η -hexane	18.4
Acetone	25.1	Isobutyl	22.9
Benzene	28.9	Methanol	22.5
η -butyl alcohol	25.4	Mercury	486.5
Carbon	27.0	η -octane	21.6
Chloroform	27.2	Oleic acid	32.5
Cyclohexane	25.2	Propanoic	26.7
Ethyl acetate	24.0	η -propyl	23.7
Ethanol	22.4	Pyridine	37.2
Di-ethyl ether	17.0	Toluene	28.5
Glycerol	63.4	Vinyl acetate	24.0
Ethylene glycol	48.4	Water	72.8

Table 2-1: Values of surface tension for different liquids in contact with air at 20°C [106].

So far the reader has been introduced to the various forces acting at the micro domain. These are graphically represented, illustrating how they scale relative to the physical dimensions of an object (Figure 2-8).

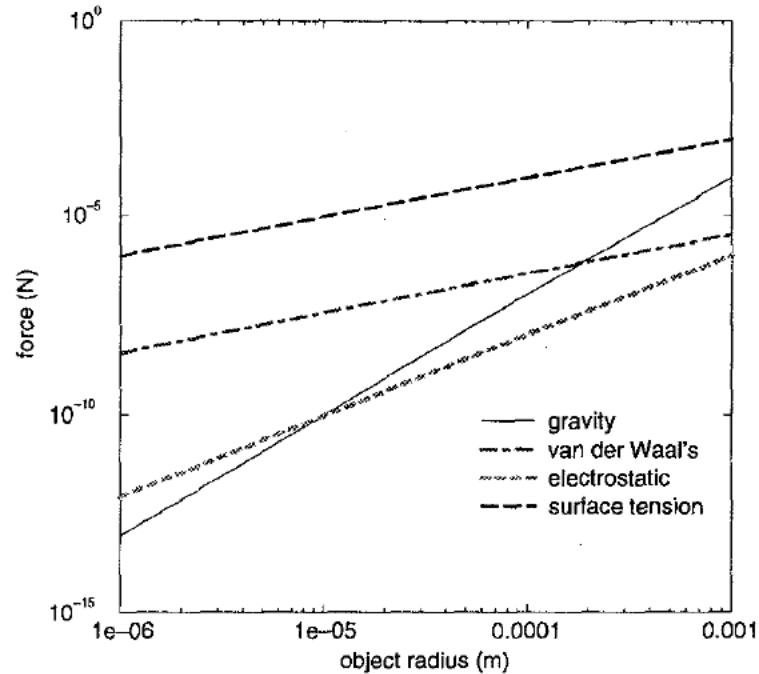


Figure 2-8: Scaling of gravitational, van der Waal's, electrostatic and surface tension forces between a silicon sphere and a conductive plate [107].

The remainder of this section is now devoted to the various laws governing liquid droplets and how these relate to their behaviour when interacting with the surrounding environment. This will include Laplace's law, surface wetting properties, Young's equation, Wenzel's law, Cassie-Baxter law, contact angle hysteresis, Bond number, and the Gibb's inequality.

2.4.5 Laplace's law

Laplace's law relates the pressure inside a droplet to the curvature of a droplet, and is fundamental when dealing with micro droplets and micro droplet interactions.

$$\Delta P = \gamma \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \quad (2-6)$$

Where γ (N/m) is liquid surface tension, and R_1 and R_2 (m) are the principal radii of the droplet. The principal radii for a spherical liquid droplet are represented in Figure 2-9.

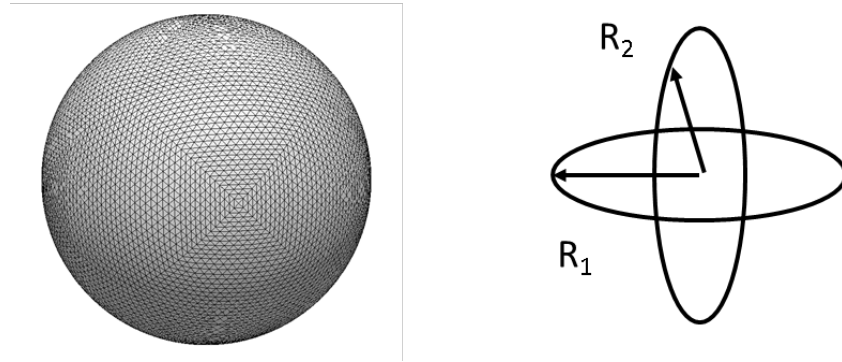


Figure 2-9: Diagram illustrating the principal radii of curvature for a spherical liquid droplet.

Laplace's law can be used for many applications including calculation of pressure in bubbles, pressure in droplets between two parallel plates, and movement of droplets between two non-parallel plates. It has also been used for direct applications such as micro flow system design where the pressure differential between two dissimilar liquid volumes can drive fluid flow [108], and modelling the evolution of the liquid bridge during evaporation between two glass spheres [109].

2.4.6 Surface wetting properties

When a liquid is placed on a solid surface two possible situations can occur. The liquid can spread out and fully wet the surface, forming a thin film, or it can partially wet the surface, forming a droplet (Figure 2-10). Which of these occurs is dependent on the properties of the liquid, the solid surface and the fluid/gas surrounding the system. The intersection of these three interfaces is known as the triple contact line (TCL) [110]. The type of liquid spreading that will occur can be determined from the spreading parameter, S :

$$S = \gamma_{SG} - (\gamma_{LS} + \gamma_{LG}) \quad (2-7)$$

Where, γ_{SG} is the solid-gas interfacial energy, γ_{LS} is the liquid-solid interfacial energy and γ_{LG} the liquid-gas interfacial energy.

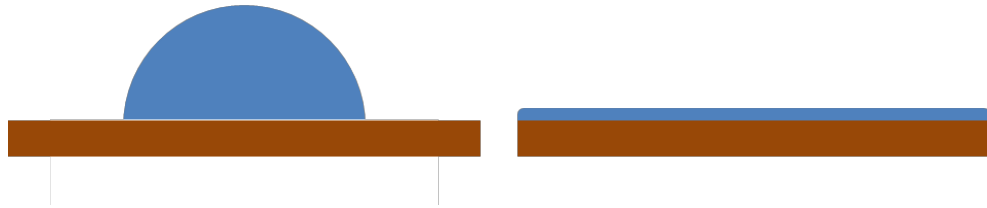


Figure 2-10: Diagram illustrating the wetting of a liquid to a solid surface. (left) partial wetting, (right) fully wetted.

The contact angle is the angle that a liquid droplet makes with a solid surface, and is measured internally of the droplet. If the contact angle with the solid is $<90^\circ$, the contact is said to be hydrophilic, whereas if the contact angle is $>90^\circ$ the contact is said to be hydrophobic (Figure 2-11). The prefix “hydro” specifically refers to water, with the generic terms being lyophilic and lyophobic, however throughout this thesis the terms hydrophilic and hydrophobic will be used.

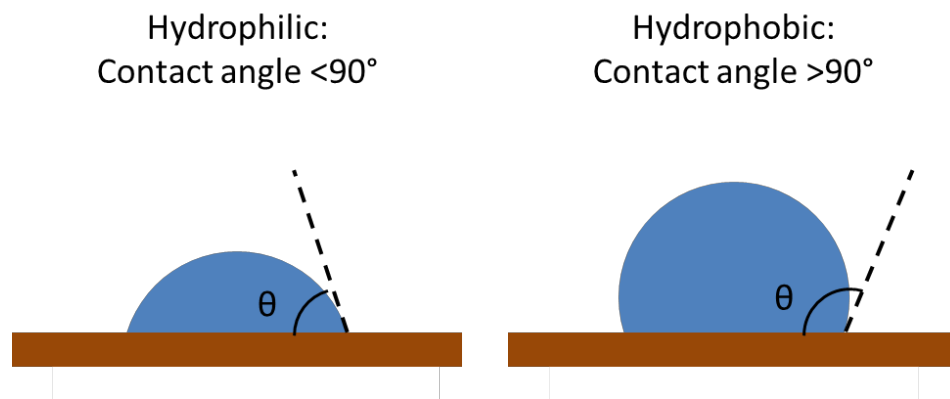


Figure 2-11: Diagram illustrating the difference between hydrophilic and hydrophobic contact.

2.4.7 Young's equation

As was previously mentioned, the point at which the solid, liquid and gas phases intersect is known as the triple contact line which can be expressed using Young's equation [111]:

$$0 = \gamma_{SG} - \gamma_{LS} - \gamma_{LG}\cos\theta_c \quad (2-8)$$

Where, γ_{SG} is the solid-gas interfacial energy, γ_{LS} is the liquid-solid interfacial energy, γ_{LG} the liquid-gas interfacial energy, and the equilibrium contact angle θ_c , as illustrated in Figure 2-12.

This is an important relation in understanding the behaviour of liquid droplets, and shows that the contact angle is determined by the interfacial energy of the three interfaces. One of the major assumptions in Young's law is that the solid surface is perfectly smooth, with zero roughness and is chemically homogenous. Real world surfaces however do not display these ideal properties, even when very careful fabrication steps are taken, and more advanced solutions are therefore needed to describe these wetting conditions which will be covered below.

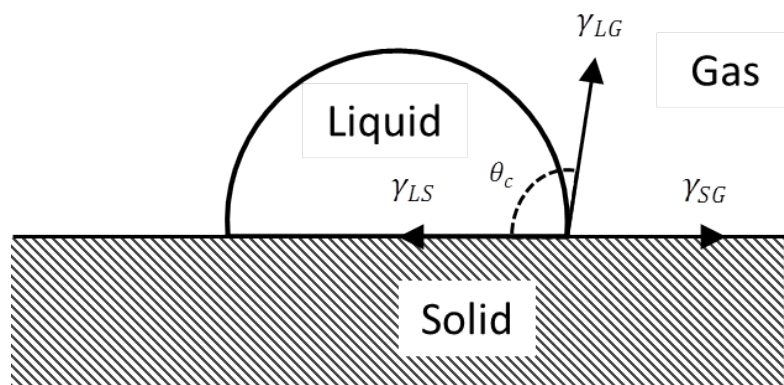


Figure 2-12: Diagram illustrating the quantities used in Young's equation (2-8).

2.4.8 Wenzel's Law

The roughness of a solid surface has a direct effect on the contact angle of a liquid, and serves to amplify the hydrophobic or hydrophilic character of the interface. In a homogenous wetting regime the liquid fills in the roughness of the solid surface (Figure 2-13). Wenzel's model, developed by Robert N. Wenzel, can be used to describe the contact angle as [112]:

$$\cos\theta^* = r\cos\theta \quad (2-9)$$

Where, θ^* is the apparent contact angle for the minimum energy state, r is the roughness ratio (which is a ratio of the true surface area to the apparent area, and is used to describe how surface roughness affects a surface), and θ is the Young contact angle for an ideal surface.

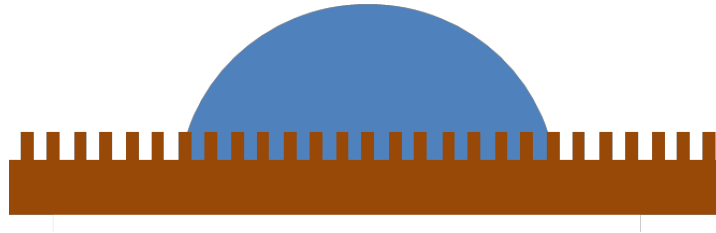


Figure 2-13: Liquid droplet in the Wenzel state, filling in the roughness of the solid surface.

An important point to note is that the scale of the surface roughness is very small in comparison to the liquid droplet dimensions, such that the molecules are interacting microscopically with a rough surface, but macroscopically with an ideal surface. If the scale of the surface roughness is equal to that of the droplet dimensions the droplet simply adjusts its position to local minima in the surface. One of the most well-known examples of this phenomenon is the lotus effect [113], which has led to the development of superhydrophobic (contact angles $>150^\circ$) surfaces [70, 74, 114, 115].

2.4.9 Cassie-Baxter Law

Cassie and Baxter conducted the same analysis as Wenzel but for chemically inhomogeneous solid surfaces rather than physical roughness. Again the same condition applies that the scale of heterogeneities must be small compared to the interaction dimensions between the liquid droplet and surface. The Cassie-Baxter law states that [116]:

$$\cos\theta^* = \sum_i f_i \cos\theta_i \quad (2-10)$$

Where, θ^* is the apparent contact angle for the minimum energy state, f_i is the surface fraction of each material, and θ_i is the contact angle for each material at a macroscopic scale.

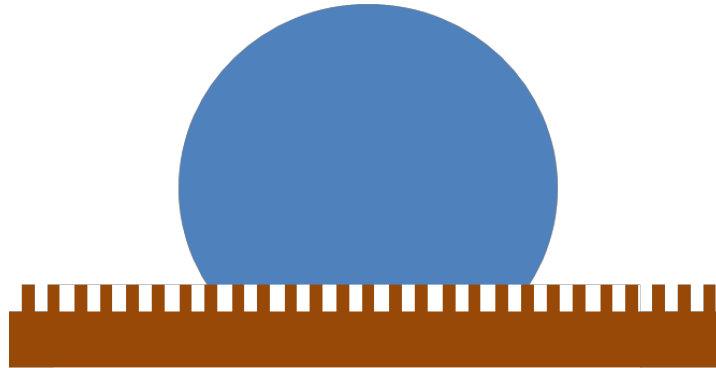


Figure 2-14: Liquid droplet in the Cassie-Baxter state sitting on top of an inhomogeneous solid surface.

2.4.10 Contact angle hysteresis

As was discussed above, the surface roughness and chemical homogeneity of a solid surface has a direct bearing on the contact angle of a liquid droplet. If a droplet is placed on an ideal planar surface the contact angle can be defined by Young's equation, however when considering real world cases the static contact angle (θ_s) is not unique. If a droplet is placed on a solid surface and its volume steadily increased via a pipette (Figure 2-15), it is observed that the contact angle increases without the triple contact line (TCL) moving. The

contact angle will continue to increase until it reaches a threshold value, θ_a , known as the advancing contact angle, after which the triple contact line will then move. The same effect can be seen in reverse when reducing the liquid volume (Figure 2-15). The triple contact line will remain pinned until a threshold value, θ_r , known as the receding contact angle is exceeded, and it will then move.

$$\theta_a > \theta_s > \theta_r \quad (2-11)$$

The difference between the advancing and receding contact angles is known as the contact angle hysteresis. Usually the advancing contact angle is much higher than the receding contact angle, with typical hysteresis values of 5-20° [110]. This effect is associated to local defects on the solid surface, either physical or chemical, which restrain the movement of the TCL [117-121].

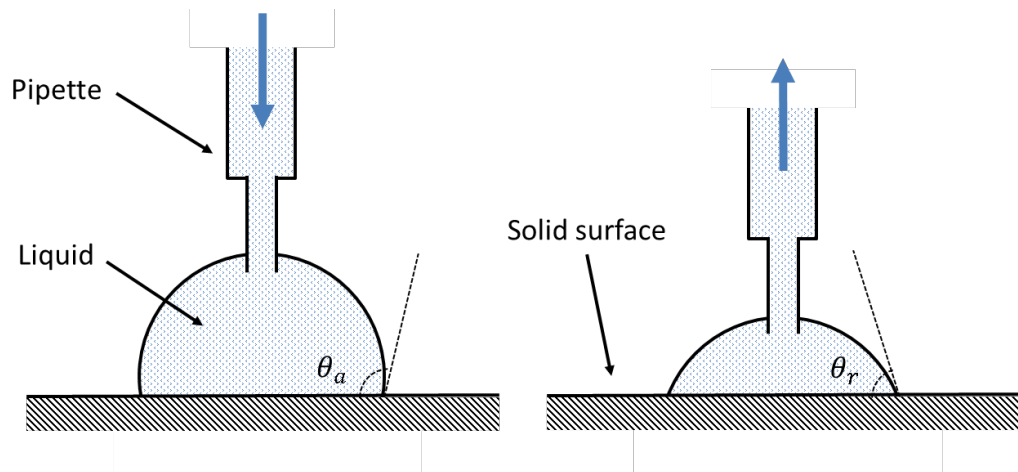


Figure 2-15: Diagram illustrating the difference between advancing (θ_a) and receding (θ_r) contact angles of a liquid droplet on a solid surface caused by hysteresis.

2.4.11 Bond number

The Bond number, or Eötvös number, is a non-dimensional number which measures the significance of surface tension forces compared to body forces, and is used to determine the shape of droplets or bubbles when immersed in another fluid [122]:

$$Bo = Eo = \frac{\Delta\rho g L^2}{\gamma} \quad (2-12)$$

Where, $\Delta\rho$ (kg m^{-3}) is the difference in density between the two fluids, g (m/s^2) is the acceleration due to gravity, L (m) is the characteristic length (typically the droplet radius), and γ (N/m) is the surface tension.

A high Bond number indicates that the system is relatively unaffected by surface tension, whereas a low number (typically less than 1) indicate that surface tension forces dominate.

The capillary length is a characteristic length scale between two fluids subject to gravitational and surface tension forces. If a system has a characteristic length below that of the capillary length it is said to have a low bond number. The capillary length is a ratio of the Laplace pressure to the hydrostatic pressure and is defined as [9]:

$$\lambda_c = \sqrt{\frac{\gamma}{\Delta\rho g}} \quad (2-13)$$

Where, γ (N/m) is the surface tension, $\Delta\rho$ (kg m^{-3}) is the relative fluid density and g (m/s^2) is acceleration due to gravity.

A droplet whose largest dimension is smaller than the capillary length will have a shape that resembles a spherical cap, whereas a droplet larger than the capillary length (high Bond number) will be flattened due to gravity (Figure 2-16).

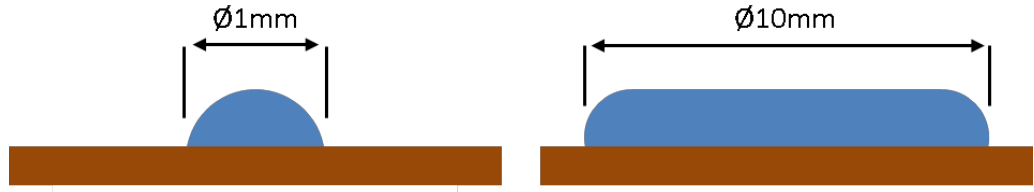


Figure 2-16: Diagram illustrating the effect of capillary length on droplet shape. (left) 1mm diameter droplet (low Bond number) resembles a spherical cap, (right) 10mm diameter droplet (high Bond number) flattened by gravity.

2.4.12 Gibbs inequality

As discussed earlier in the chapter, the occurrence of defects on a surface can result in halting droplet movement via pinning of the triple contact line (TCL). The same effect can occur along an edge and act to pin the droplet in place, preventing any further movement. Structures that control liquid spreading through halting the movement of the TCL at a defined edge are based on the mathematical inequality presented by Gibbs [123]:

$$\theta_c < \theta < (180^\circ - \alpha) + \theta_c \quad (2-14)$$

Where, θ is the contact angle of the droplet, θ_c is the Young's contact angle, and α is the angle of the sharp edge, see Figure 2-17.

This states that as long as the liquid droplet's contact angle does not exceed the Young's contact angle for a planar surface plus the angle of the edge geometry, the TCL will remain pinned to the edge. It is important to note however that the Gibbs inequality assumes that the edges are perfectly sharp. This of course is physically impossible, and the actual edge geometry will display some form of radius which is heavily dependent on the manufacturing process used to produce the structures.

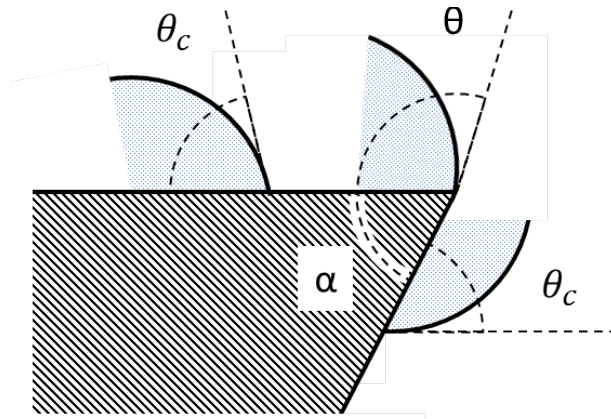


Figure 2-17: Spreading of a liquid droplet meeting a sharp edge as described by the Gibbs inequality, equation (2-14).

2.5 Computational analysis for microfluidics

As is evident from the previous section discussing the physics affecting liquid droplet micro assembly, it is extremely difficult to model the behaviour of these assembly processes using purely analytical solutions for anything but highly simplified cases. It therefore becomes apparent that in order to gain a realistic representation of the process numerical computational analysis of the system is necessary. There are a number of different software tools available that deal with computational analysis of systems and these will be described below, with their ability to handle microfluidic problems discussed.

Computer Aided Design (CAD) is the use of computer software to create 2D drawings or 3D models. It is used by designers in a wide range of fields for the creation, modification, analysis, and optimisation of a design. There are many different types of CAD software available, however the typical industrial packages are based on 3D parametric solid modelling such as PTC Creo, Solidworks, and CATIA [124-126]. These are purely design packages; however some feature computer aided engineering (CAE) modules which can be purchased as aftermarket add-ons, or as entirely separate software solutions. These allow the design engineer to carry out analysis on a designed component or assembly such as multibody dynamics (MBD), static analysis, or kinematic analysis. They do not however offer analysis for fluid flow, or fluid behaviour and dedicated software is needed which will be discussed below.

Finite element analysis (FEA) is another branch of CAE which can be a module of a CAD package or a standalone software package. It allows the analysis of complex problems by dividing the system into many small elements (a mesh) which can be individually easily calculated. The problem is usually based on a physical system and therefore specific laws can be applied to the relevant elements to accurately capture the behaviour of the system. FEA is a powerful analysis tool however the computational time is directly related to the mesh refinement, where a finer mesh is needed to accurately model the system behaviour. This makes the software computationally intensive, and many problems are therefore run on a high performance computer (HPC) network to speed up the process.

Computational fluid dynamics (CFD) is a branch of fluid dynamics that deals with the numerical modelling of fluid flow. It involves the analysis of interactions between liquids, or gases and solid surfaces which are defined through boundary conditions. Similar to FEA packages described above, CFD is also a computationally intensive task usually requiring the use of a HPC network.

Surface Evolver (SE) is a free-to-use software package developed by Kenneth Brakke used to model surfaces shaped by surface tension and other energies. The program uses a gradient decent method to evolve surfaces to a minimum energy state subject to a number of user defined energies. These include surface tension, gravitational energy, squared mean curvature, user-defined surface integrals, or knot energies. The program is also capable of utilising volume constraints, boundary constraints, boundary contact angles, gravity and constraints expressed as surface integrals. Unlike other FEA packages SE is only concerned with surfaces therefore only the surface needs to be meshed. Due to not having to account for elements within bodies the computational time is significantly lower than other packages. Surface Evolver has been used to model such things as solder joints used for out-of-plane folding of MEMS structures [96, 127-130], investigation of liquid droplet contact angles on inclined surfaces [131], modelling chip alignment for individual degrees of freedom (DOF) [85], coupled DOF [132], modelling the effect of defects in

binding sites [84, 133], and the investigation of hydrophobic surface patterning to prevent assembly defects [134].

2.6 Summary and identification of knowledge gaps

This chapter has introduced the reader to the concept of micro components along with the current assembly and handling strategies utilised to combine them into finished product assemblies. An overview of microfluidics was presented, specifically focusing on self-assembly applications. A review of the physics present during liquid droplet alignment tasks was introduced, before proceeding to commonly used computational analysis tools and their applicability to this work. The literature review has led to the identification of the following knowledge gaps:

2.6.1 *Lack of a methodology for the design of additively manufactured components for microdroplet alignment*

Additive manufacturing offers the design flexibility to easily incorporate features such as binding sites for liquid alignment, and many AM techniques can produce parts that are small enough to make traditional manual handling a challenge. Liquid droplet based assembly techniques are well documented for a range of industries and production methods, but there are no studies that specifically consider the application of additive manufacturing. For these reasons a methodology is needed for the design and manufacture of additively manufactured structures suitable for microdroplet alignment applications. This will allow the manufacture and experimental investigation of additively manufactured structures to assess their performance.

2.6.2 *Lack of intuitive numerical modelling tools to aid in the design of structures for microdroplet component alignment*

Surface Evolver is free-to-use software that allows the investigation of surfaces shaped by surface tension and other forces. One of the strengths of Surface Evolver is that it is not designed for a specific task and so is highly flexible. This however means that its use in the literature is highly diverse. A number of researchers have used the software for modelling the alignment of components

using liquid surface tension, however the cases presented were for small integrated circuit dies of a few hundred microns and are therefore not applicable to the scale of the components investigated in this thesis. There is therefore a need for additional simulations to be performed to investigate components in the millimetre range.

Surface Evolver requires users to generate data files for simulations by defining the model in a text file via coordinates. This makes the definition of complex geometries within Surface Evolver extremely difficult, and the process of component optimisation laborious. All of these factors mean that the software is highly unlikely to be used outside of a purely research environment. There is therefore a clear need for integration of Surface Evolver derived data into a well understood computer aided engineering (CAE) environment to allow the optimisation of structures for microdroplet alignment in an industrial design environment.

2.6.3 Lack of numerical model to assess the effect of non-idealised edge geometries

The Surface Evolver models presented in the literature simplify the structures to have idealised edge geometries and that the assembly liquid remains pinned to both the binding site and component. Many manufacturing processes are unable to create these highly sharp edges and the existing models do not therefore adequately represent the behaviour of the alignment process for these non-idealised structures. Additionally there is a lack of analytical approach as these tend to be limited to simple geometries under specific conditions.

The creation of new Surface Evolver models is therefore needed which examine the effect of different edge geometries on the liquid droplet behaviour during self-alignment applications. This is needed to provide a more realistic representation of the physical system and allow informed design decisions to be made relating to alignment tasks, for manufacturing processes which may produce these non-idealised edge geometries.

Chapter 3

3 RESEARCH METHODOLOGY

Having previously identified the knowledge gaps from the current literature and defined the project objectives, this chapter explains how they will be addressed in the context of the thesis. A range of research activities including experimental work and modelling were planned, which are discussed in detail through the following chapter. The specific research needed to meet the stated objectives is presented in the research approach. Following this the assumptions and limitations present in the work are explained. The chapter is concluded with technical details of the experimental methods and fabrication processes used in the project.

3.1 Research Approach

The following subsections describe the research activities undertaken to achieve the aim and objectives outlined in Chapter 1. The justification for the research methods is presented below while the actual experimental work and results are detailed in chapters 4 - 8 of the thesis.

3.1.1 *Characterise a suitable additive manufacturing process for the production of liquid alignment binding sites*

The requirement for a successful binding site is its ability to retain the assembly liquid within a defined region. This can be achieved either through a contrast in wettability between surfaces, or by creating a physical obstacle to liquid motion. In the latter case, it is necessary that the structure have a well-defined edge, free from defects. Additive manufacturing offers the design flexibility to easily incorporate features such as binding sites for liquid alignment, additionally many AM techniques can produce parts that are small enough to make traditional manual handling a challenge. A range of binding site geometries and configurations were manufactured using a projection microstereolithography process to establish design rules for the fabrication of functional structures. Fabrication was carried out using an EnvisionTec Perfactory using R11 resin.

3.1.2 *Investigate the effect of binding site edge geometry on the ability to control liquid spreading, and its role as an early indication of assembly reliability*

The containment of the liquid droplet to the binding site is of key importance to alignment applications. The liquid droplet behaviour when it encounters the binding site edge is determined by the Gibbs inequality (see chapter 2, section 2.4.12). An experimental investigation was conducted to establish the contact angle of liquid droplet on the manufactured binding sites. A series of challenging assembly tasks were carried out to assess the manufactured binding sites' ability to offer precision alignment for components.

3.1.3 *Define a model to examine the effect of binding site edge geometry on the liquid droplet during assembly*

The existing models presented in the literature simplify the binding site geometry and assume that it has perfectly sharp edges. An additional assumption is that the liquid droplet remains pinned around the perimeter of both the binding site and component faces throughout the assembly process. Models were created using the free-to-use software Surface Evolver to carry out numerical simulations which examined binding site edge radius, and binding site undercuts and the role these play in liquid droplet alignment.

3.1.4 *Define a series of models expressing the forces generated by a liquid droplet under typical self-assembly conditions and how this can be applied in a design context*

The response of liquid droplets during alignment applications need to be established for the types of structures investigated in this thesis so they can later be applied in a design context. Models were created using Surface Evolver and used to simulate a component while under different misalignment conditions which constituted the six degrees-of-freedom of the component.

3.1.5 *Demonstrate the application of the above models and insights in the design of components for a micro component alignment test case*

Surface Evolver is a powerful tool for modelling surfaces shaped by surface tension and other forces. It is able to handle simple geometries however is not

suitable for complex geometries or design studies. For these cases the integration of the Surface Evolver data into a more intuitive CAE package to allow design optimisation is desirable. The above models and insights were used to design components for a micro component alignment test case. The case presented was that of a high aspect ratio component. A model was created using Surface Evolver and compared to a simple analytical solution, and experimental investigation. The numerical solution derived from Surface Evolver was then integrated into a commercial CAE package to demonstrate its feasibility as a design tool for component optimisation.

3.2 Instruments and experimental procedures

In the following section the experimental procedures are detailed as well as technical details of the equipment used. While all of the instruments used are commercially available they have been described in order to present a clear picture to the reader. Workshop machinery used for the manufacture of any test rigs is not described here, along with basic metrology devices such as Vernier callipers, micrometres, protractors, scales etc.

3.2.1 *Component manufacture*

Components were manufactured using projection-micro-stereolithography (PMSL), a solid free-form fabrication technique based on controlled solidification of a liquid, light-sensitive resin when exposed to a light source (photopolymerisation). Using an LCD or Digital Micromirror device (DMD) the polymer is successively exposed and solidified in 25 μm layers to construct 3-dimensional geometries according to data from an STL file. An EnvisionTec Perfactory® Mini-Multi lens projection stereolithography machine (Figure 3-1) using EnvisionTec R11 rapid prototyping material was used. This resin was chosen due to its achievable layer thickness and well established curing behaviour in the build process. Projector brightness was calibrated to 600 mW/dm^2 with exposure time of 4.0 seconds/layer (standard range), at a layer height of 25 μm . Resolution was set to 1050 x 1400 pixels (SXGA+),

equivalent to a pixel size of 5 μm in X,Y-direction. The manufacturing parameters are summarised below in Table 3-1.

Wavelength:	380-480 nm
Power:	600 mW/dm ²
Exposure time:	4 sec (standard), 20 sec (burn-in)
Resolution:	1050 x 1400
Pixel size (X,Y):	5 x 5 micrometres
Layer thickness (Z):	25 micrometres

Table 3-1: Process parameters for component manufacture.

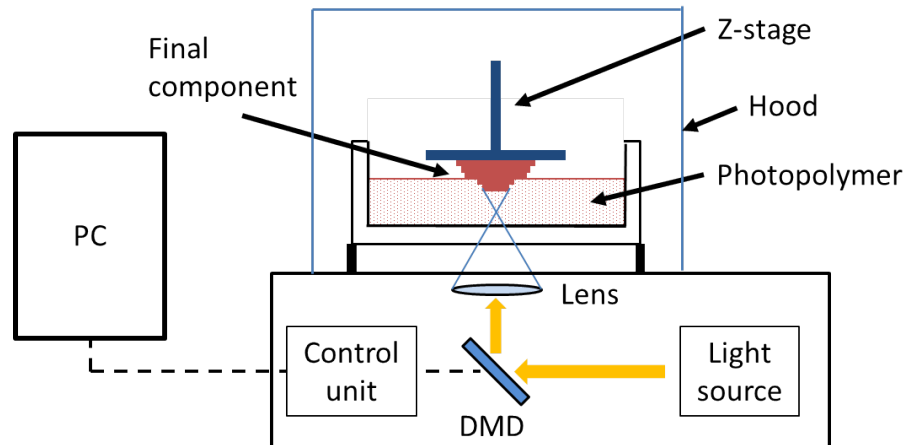


Figure 3-1: Schematic of EnvionTec Perfactory Mini-Multi lens projection stereolithography machine

3.2.2 Component test geometries

Structures were designed to examine the effect of edge geometry on the ability to pin the TCL of a spreading liquid droplet. Since droplets have a spherical shape when in their lowest energy state circular binding sites were selected.

This was also due to their axial-symmetry and ease of manufacture. Components containing test arrays of Ø0.4, 0.5, 0.6, 0.75 and 1 mm circular binding sites were manufactured in the aforementioned method (see section 3.2.1). Test arrays containing square binding sites of 0.5 x 0.5 mm and 1 x 1 mm were manufactured using the same method. Each feature was located in a 0.1 mm deep hole, while being 0.1 mm tall, resulting in the binding site surface being flush with the surface of the bulk material of the test array. Due to the absorption of light, the minimum achievable layer thickness was 25 µm. For practical applications it is desirable for the binding site to have a shallow profile so as not to interfere with the overall form or function of the component. A binding site height of 100 µm was considered suitable for producing the range of edge geometries while limiting layer numbers and therefore reducing the likelihood of production defects occurring. This corresponded to a binding site height of 4 build layers. The diameter of the “trench” surrounding each structure was Ø1.5 mm for circular binding sites, and 2 x 2 mm for square binding sites. Rendered images of the binding site test array as well as a SEM image of the fabricated structure can be seen in Figure 3-2. Close-up of the binding site edge has been provided for clarity. This design was chosen in order to protect the edge of the binding sites from damage during the handling and cleaning process and to give sufficient clearance between the structures and surrounding bulk material to prevent any interaction when applying the liquid. A cross-sectional example of the binding site geometry used for this work can be seen in Figure 3-3.

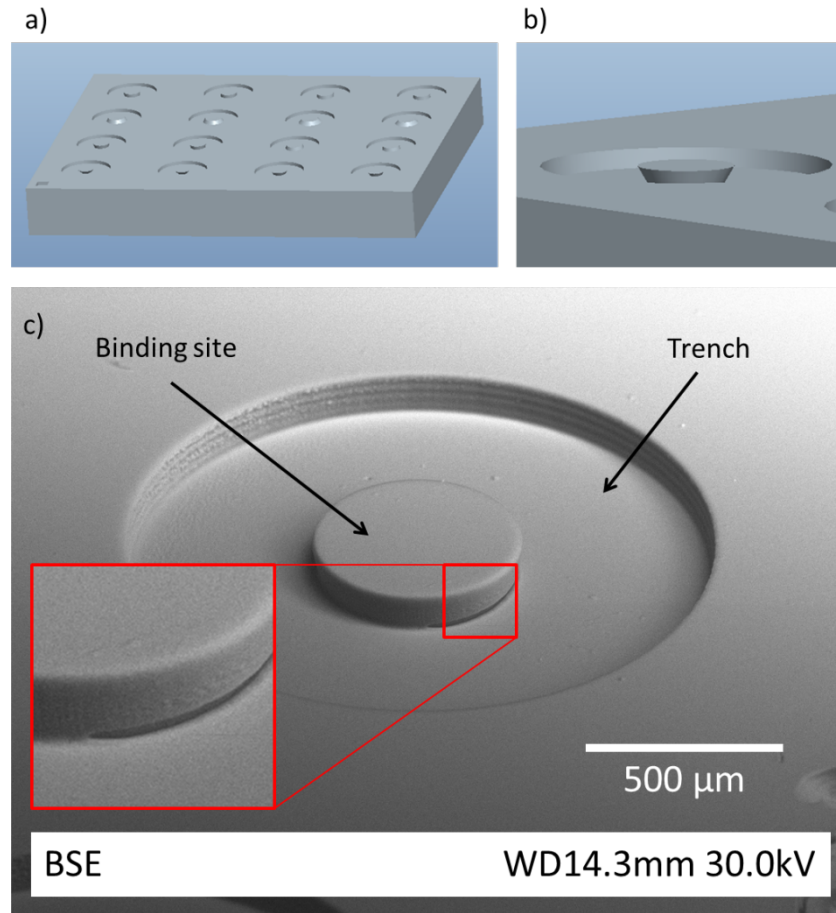


Figure 3-2: a) Rendered image of test component with array of Ø0.5 mm circular binding sites, b) Rendered image of a single binding site with 45° nominal edge geometry, c) SEM image of Ø0.6 mm circular binding site with 60° nominal edge geometry.

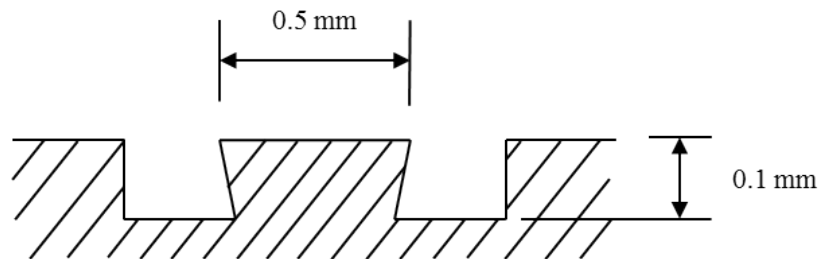


Figure 3-3: Cross-sectional diagram of binding site geometry for Ø0.5 mm circular binding site.

The structures' sharp edges were altered to investigate acute (undercut) angles, and obtuse (chamfer) angles, as illustrated in Figure 3-4. Edge geometries of 45-135° were manufactured for all above mentioned structures in 15°

increments. Additional angles of 85 and 95° were manufactured for Ø0.5 and 1 mm circular binding sites as the area around 90° was believed to be a key angle of interest. All binding sites were inspected after manufacture under an optical microscope before carrying out further experiments.

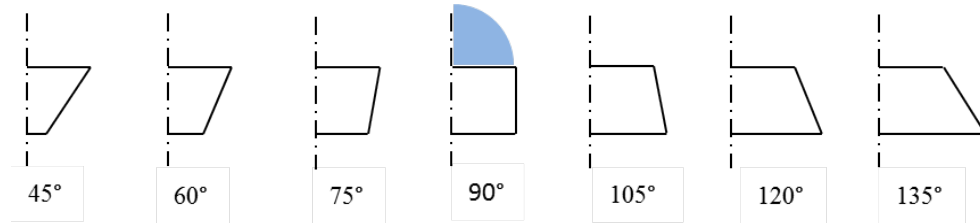


Figure 3-4: Nominal edge geometries of topographical structures. Blue region indicates liquid droplet placed on top surface of the structure.

3.2.3 Component preparation and cleaning procedure

Due to the nature of the manufacturing process it is necessary to incorporate support structures into the design of components. This is necessary when the component has significant overhanging features or large hollow structures that need supporting as the layers are successively cured during the build process. The inclusion of support structures is also required when producing individual parts which need to be separated from the base burn-in layer. Support structures are carefully removed following the cleaning process using a scalpel.

Parts were cleaned post build in an ultrasonic isopropanol alcohol bath for 3 minutes, followed by a second isopropanol solution for a further 3 minutes, and allowed to dry in air. All components were manufactured in a temperature controlled laboratory at 21° Celsius.

3.2.4 Measurement of component mass

Component mass was determined by weighing the components manufactured for the experimental investigation of the tipping case study (section 8.2.3) using an Adam Equipment PW254 laboratory balance. The components were rectangular based prisms of 2 x 2 mm cross sectional area, with varying lengths of 8.5 – 12.5 mm in 1 mm increments, and circular based prisms of cross

sectional diameter 2.26 mm, with varying lengths of 8.5 – 12.5 mm in 1 mm increments (20 components total).

Components used throughout the thesis were viewed under an optical microscope and their dimensions measured in ImageJ. All components were found to exhibit shrinkage, with measured dimensions being no more than 5% below the nominal values (Figure 3-5).

Component density was estimated by dividing the measured component mass by the measured component dimensions. The density of components produced using the EnvisionTec Perfactory was found to be 1209 kg.m^{-3} with a standard deviation of 18 kg.m^{-3} .

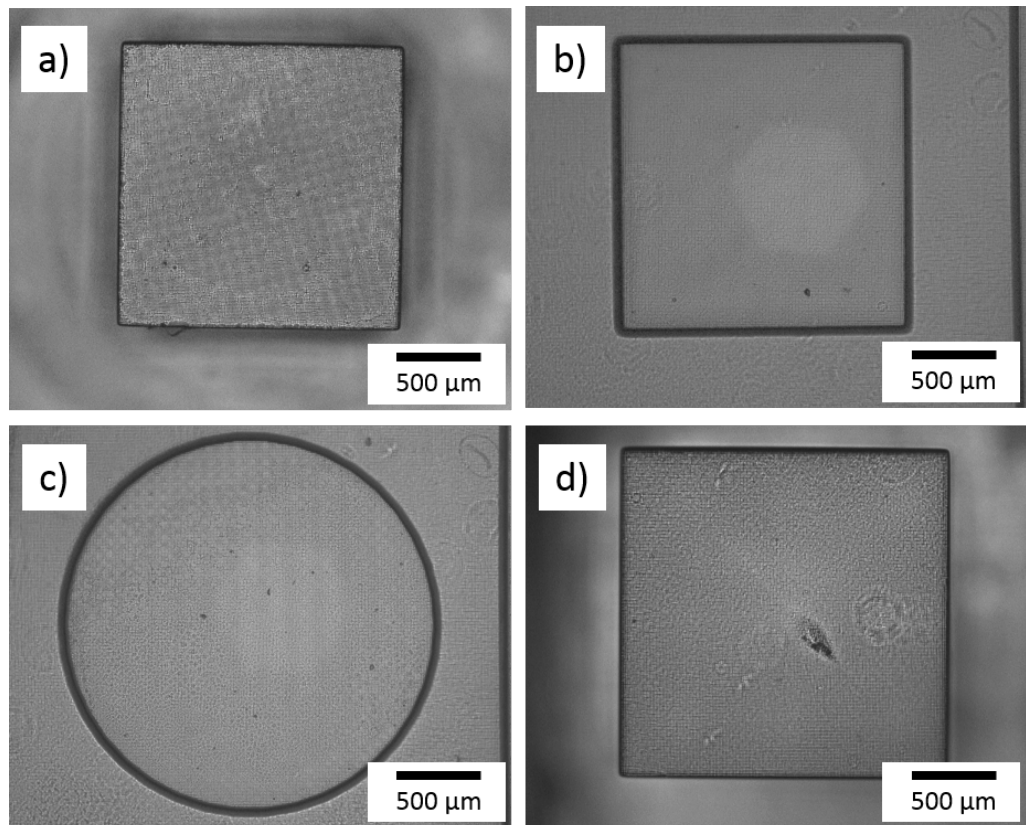


Figure 3-5: Optical microscope images of components produced on the EnvisionTec Perfactory. a) Indenter tip, dimensions 1.75 x 1.75 mm, b) Square binding site, dimensions 1.75 x 1.75 x 0.1 mm, c) circular binding site, dimensions $\varnothing$ 2.26 x 0.1 mm, d) Rectangular prism component, dimensions 2 x 2 x 8.5 mm.

3.2.5 General experimental setup

Experiments were conducted in an air-conditioned laboratory environment at 20° Celsius. Before testing parts were cleaned in an ultrasonic isopropanol alcohol bath for 3 minutes, followed by a second isopropanol solution for a further 3 minutes, and allowed to dry in air. Components were mounted on an X-Y precision stage and viewed under an optical microscope with a JVC TK-C1381 CCD mounted camera. Data were captured using a Hauppauge Win-TV-HVR-1900 interface with post process image analysis conducted using the ImageJ software package. Liquid water droplets were applied to the binding sites using a digital timed precision fluid dispenser TS-250 from Adhesive Dispensing Ltd (Figure 3-6). A 3cc syringe barrel was used in conjunction with a 34 gauge blunt end dispensing tip (Figure 3-7). The liquid used for the experiments was distilled water with surface tension, $\gamma=72.8 \text{ mN m}^{-1}$.

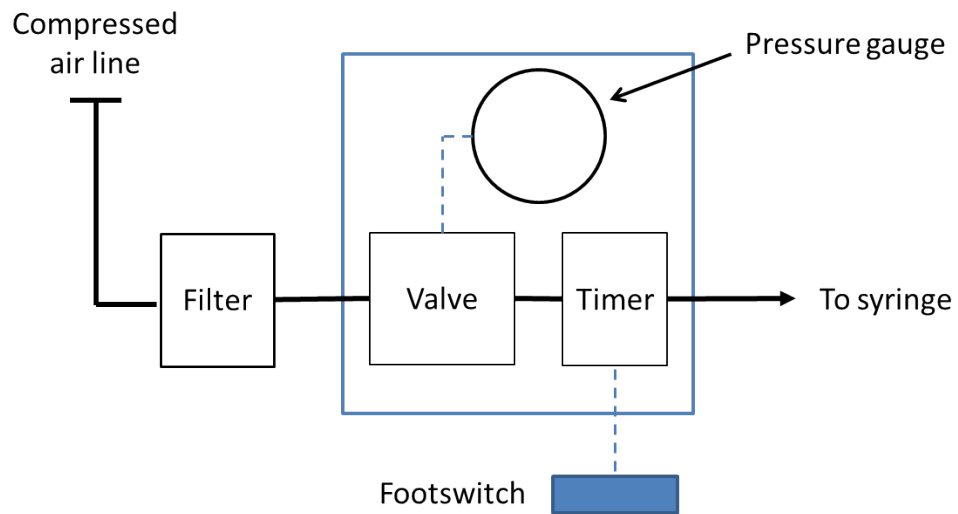


Figure 3-6: Schematic of TS-250 precision fluid dispenser from Adhesive dispensing Ltd.

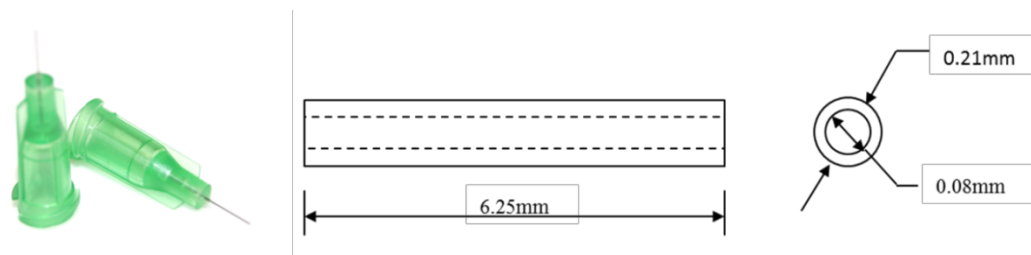


Figure 3-7: 34 gauge blunt end dispensing tip used for liquid droplet dispensing.

Scanning Electron Microscope (SEM) images presented in this thesis were captured using a Hitachi S-2600N SEM operating in low vacuum mode at 30kV acceleration voltage.

3.2.6 *Contact angle measurements*

In order to establish a benchmark by which to compare the effect of the structures, a background reading for the static contact angle of water on the polymer material used by the additive process, needed to be established. To do this two flat plain substrates of dimensions 10 x 12 x 2.5 mm were manufactured using the fabrication method described in section 3.2.1. A single liquid water droplet was dispensed onto the surface using the fluid dispenser described in 3.2.5. Droplets were viewed from the side using an optical microscope with a JVC TK-C1381 CCD mounted camera mounted perpendicular to the substrate surface. Data were captured using a Hauppauge Win-TV-HVR-1900 interface, with contact angles analysed post experiment in ImageJ software using the public domain Low bond axisymmetric drop shape analysis (LB-ADSA) plugin, developed by A. Stalder [178]. 15 measurements were performed and the contact angle of water on the plain polymer substrate was determined to be 70° with a standard deviation of 3°.

3.2.7 *Liquid volume measurements*

Liquid volume measurements were performed under an optical microscope with a JVC TK-C1381 CCD mounted camera. Data were captured using a Hauppauge Win-TV-HVR-1900 interface with post process image analysis conducted using the ImageJ software package. Using the experimentally determined static contact angle (section 3.2.6), droplet volumes were calculated by measuring the droplet wetted area from the top-down image prior to component placement using the following formula [108]:

$$V = \frac{\pi(2 - 3\cos\theta + \cos^3\theta)}{3} \frac{a^3}{\sin^3\theta} = f(\theta) \frac{a^3}{\sin^3\theta} \quad (3-1)$$

Where a is the radius of the droplet in contact with the binding site, and θ is the contact angle (illustrated in Figure 3-8).

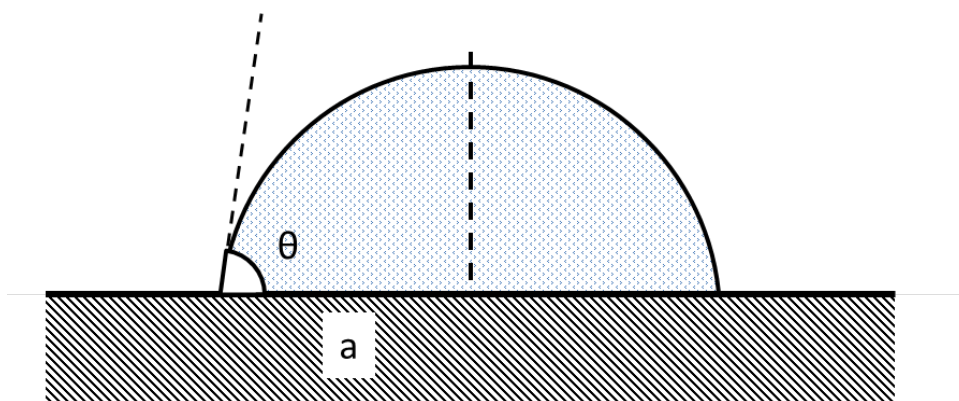


Figure 3-8: Diagram illustrating the parameters used in equation (3-1) to calculate the volume of a spherical cap.

It is important to note that this method of volume calculation assumes that the droplet is a spherical cap, and is therefore only suitable for droplets which have a low Bond number, where gravitational effects are negligible and does not influence the droplet shape (section 2.4.11). It should also be noted that this method is only suitable where the droplet exhibits a hydrophilic contact with the solid surface. When viewed from above the major diameter is therefore the triple contact line in contact with the solid surface.

The error in estimation of the liquid volume was determined by measuring the area of a liquid droplet when viewed from above 10 times in ImageJ. When used in equation (3-1) and assuming a contact angle of 70° , the average liquid volume was found to be 213 nl with a standard deviation of 2.4 nl.

A second estimation of the error in liquid volume measurement was performed based on the contact angle of the liquid droplet with the surface. In section 3.2.6 the contact angle of a liquid water droplet on a plain polymer substrate was measured 10 times, which revealed a contact angle of 70° with a standard deviation of 3° . For the same droplet area as measured above, one standard deviation in the contact angle either side of the mean resulted in equation (3-1)

reporting a liquid droplet volume of 198 nl and 229 nl for 67° and 73° contact angles respectively.

3.2.8 *Constraint of liquid spreading*

The ability of the designed binding sites to contain liquid droplets was experimentally investigated. A single liquid droplet was dispensed onto the centre of the binding sites using the same precision fluid dispenser described above in section 3.2.5. The droplets volume was then incrementally increased by applying additional liquid to the original droplet. After each application the droplet was allowed to stabilise and reach equilibrium before proceeding with further applications. Droplets were applied to the original droplet up to the point of collapse when the liquid escaped the binding site and was no longer constrained. The liquid was then removed from the surface using a dry compressed inert gas. Each binding site was manufactured twice, and the experiment was conducted 5 times for each site, resulting in 10 data points (N=10). Data were captured using an optical microscope with a JVC TK-C1381 CCD mounted camera and Hauppauge Win-TV-HVR-1900 interface. The optical microscope was positioned perpendicular to the binding site surface so as to capture the profile of the liquid droplet. Contact angles were analysed post experiment in ImageJ software using the public domain Low bond axisymmetric drop shape analysis (LB-ADSA) plugin (Figure 3-9).

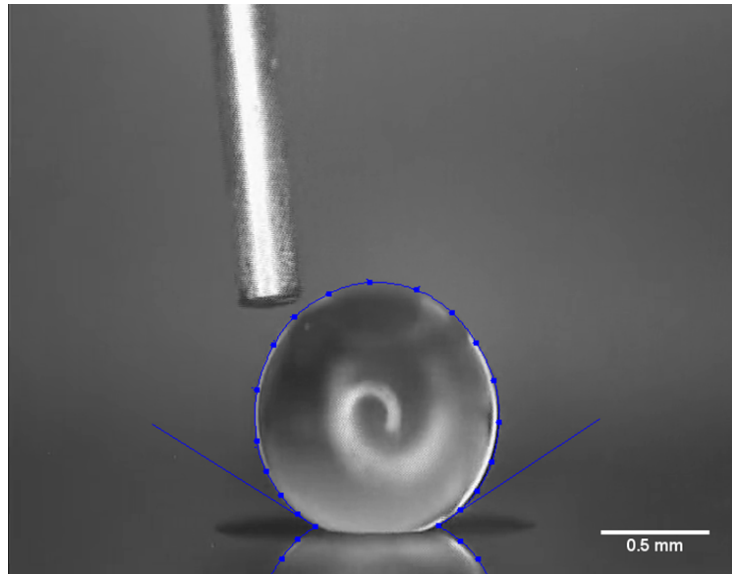


Figure 3-9: Measurement of liquid water droplet contact angle placed on a $\text{Ø}600\text{ }\mu\text{m}$ circular binding site using the LB-ADSA plugin within ImageJ.

3.2.9 *Self-assembly experiments*

Self-assembly tasks were performed by applying a single liquid water droplet to the centre of the binding site using the same precision fluid dispenser described in section 3.2.5. Components were manipulated by hand using tweezers and brought into contact with the liquid droplet before release. Components were allowed to reach their equilibrium position which was then analysed post-experiment by measuring the difference between component and binding site centres using ImageJ software.

The self-assembly experiments were performed under an optical microscope with a JVC TK-C1381 CCD mounted camera. Data were captured using a Hauppauge Win-TV-HVR-1900 interface with post process image analysis conducted using the ImageJ software package.

Binding site central coordinates were measured in ImageJ using an image captured prior to liquid droplet deposition. Final component central coordinates were measured in ImageJ using an image captured after the self-assembly operation. The difference between the two coordinate centres was then used to determine the final component misalignment from the binding site.

3.2.10 *Experimental observations of liquid droplet response*

A novel set of experiments to investigate the performance of additively manufacturing binding sites to constrain liquid water droplets were performed using an Agilent G200 nanoindenter at the University of Leicester.

The tip of the indenter was replaced with a custom tip designed using PTC Creo CAD package and then additively manufactured using the EnvisionTec Perfactory. Rather than the traditional tip shape of a nanoindenter which is used for making indents, the replacement tip (which will now simply be referred to as the indenter tip) featured a 1.75 x 1.75 mm square binding site, which was the maximum achievable size based on the geometry of the indenter equipment. The rendered CAD image and wireframe images of the designed indenter tip can be seen in Figure 3-10.

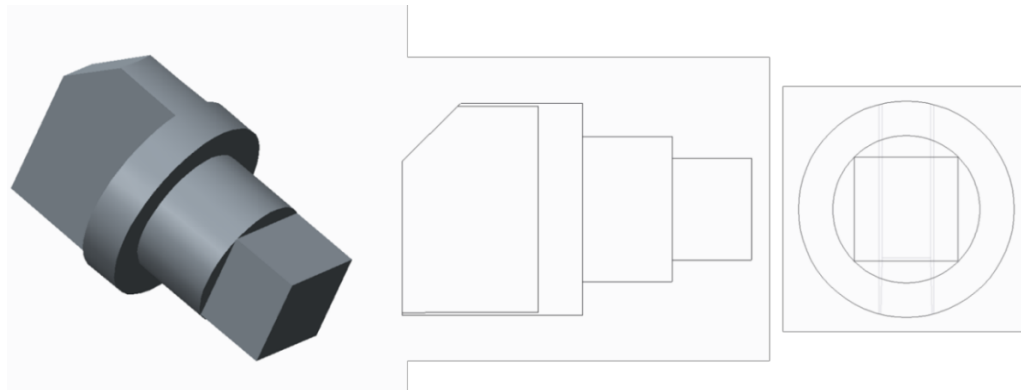


Figure 3-10: Rendered CAD image and wireframe models of indenter tip.

A test array containing 1.75 x 1.75 x 0.1 mm square binding sites was manufactured with undercut edge geometries of 80°. The binding sites were surrounded by 3 x 3 mm trenches. A measurement strategy was developed within the Testworks 4 indenter software in order to carry out the work. This began with a fast travel speed (50,000 nm/s) to a known raw displacement value above the liquid droplet. The indenter tip then proceeded at a slow travel speed (5,000 nm/s) until a force rate of 50 N/m was detected which indicated contact with the liquid droplet. At this point the indenter tip would travel a further 50 µm at the slow travel speed before retracting the indenter tip. In the

case of a failed detection of the liquid droplet a safety stop was introduced that if the raw load exceeded 81 μN (indicating a collision with the binding site) the test would be aborted and returned to the home position. A graphical summary of the measurement strategy is displayed in a flowchart (Figure 3-12). The binding site array was attached to a sample block using an SEM adhesive mount and then secured in the sample tray. Before testing a calibration procedure was performed to position the optical microscope relative to the indenter column. A second calibration was carried out in order to identify the position of the binding site surface relative to the indenter tip so that safe distances for fast travel could be determined. For the testing procedure the sample tray was moved into the loading position and a single liquid droplet of water was dispensed onto the binding site centre using the same precision fluid dispenser described in section 3.2.5. The sample tray was then moved back under the optical microscope and a 3-point coordinate measurement of the liquid droplet diameter was taken in order to calculate the liquid volume (section 3.2.7). The measurement strategy was then immediately started and results recorded in the Testworks 4 software. Following the test procedure the liquid was removed from the binding site and indenter tip using a dry compressed inert gas. The test setup along with a detailed view of the indenter tip mounted in the column can be seen in Figure 3-11.

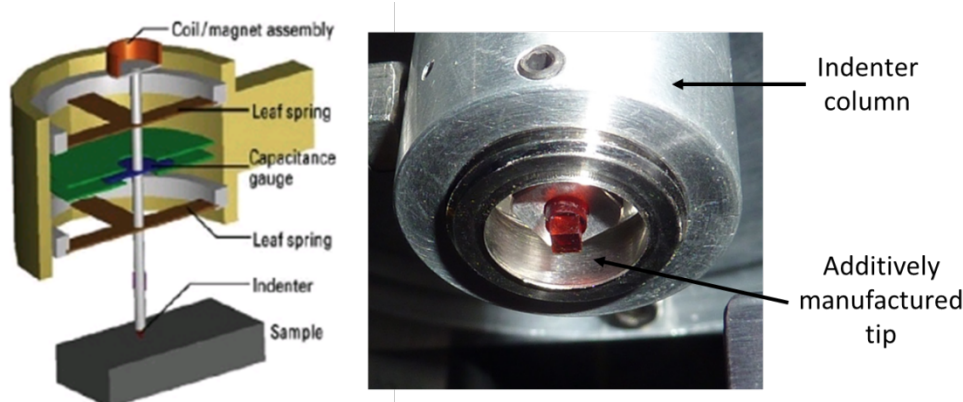


Figure 3-11: (left) Schematic of Agilent G200 [179], (right) close-up image of indenter tip fitted to column.

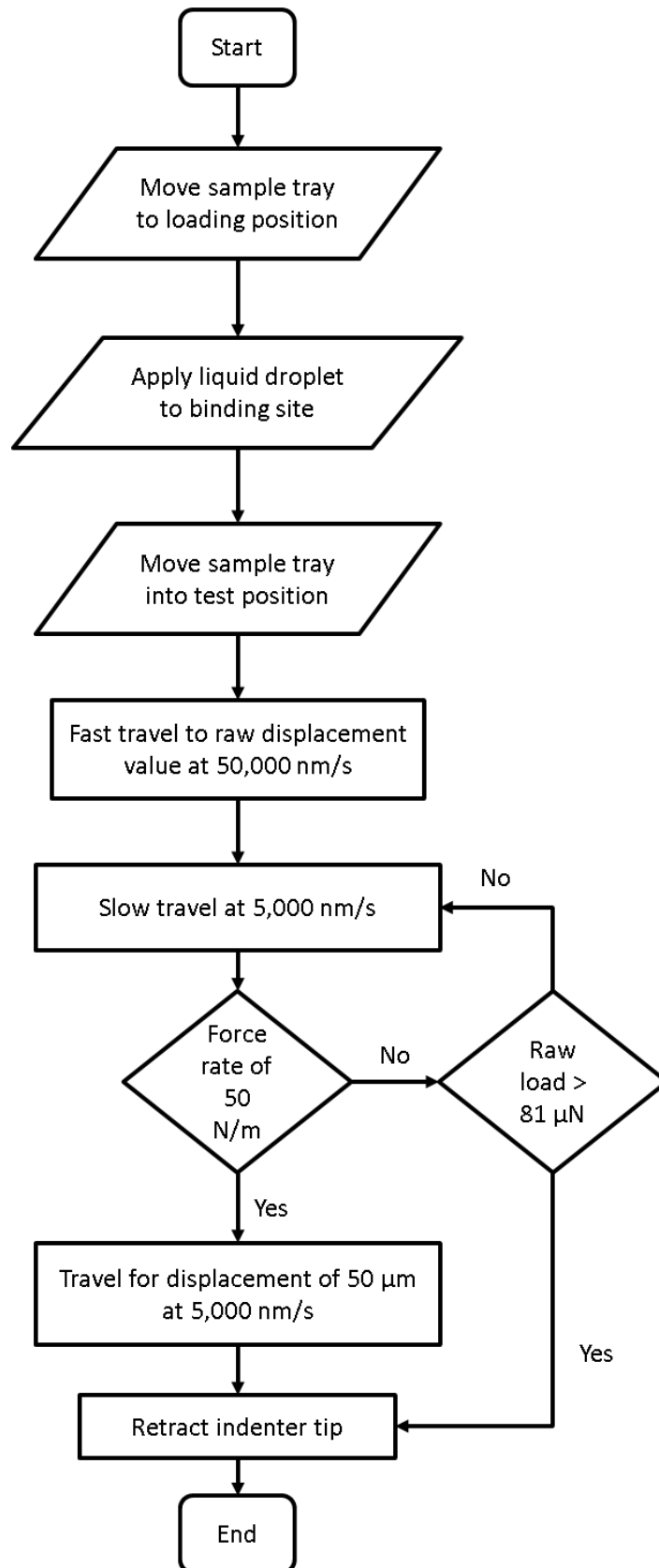


Figure 3-12: Flowchart of nanoindenter measurement strategy.

3.2.11 *Experimental investigation of high aspect ratio test case*

Investigation of the tipping of high aspect ratio structures was performed on a custom built rig. A stage with rotation about 1 axis was used to mount the binding sites. A PixeLink PL-B742F fixed focal length IEEE camera was mounted on a plate attached perpendicular to the rotating stage. This allowed the camera to rotate with the stage and view the component angle relative to the binding site at all times. The angle of rotation of the stage was viewed with a second camera, mounted on a separate plate attached to the fixed portion of the stage (Figure 3-13).

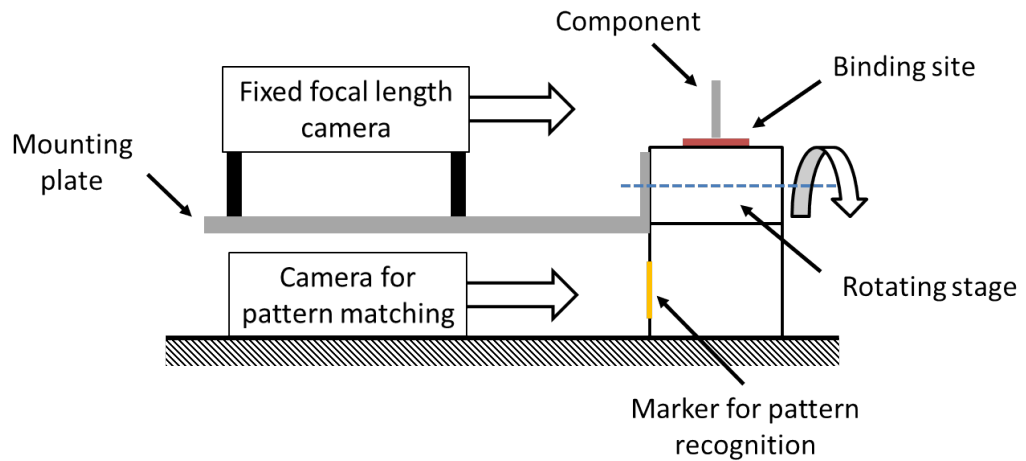


Figure 3-13: Schematic of experimental rig used for tipping experiments.

A single liquid water droplet was applied to the centre of the binding site using the same precision fluid dispenser described above in section 3.2.5. The component was then placed on the liquid droplet by hand using tweezers, and allowed to settle. The stage was then mechanically rotated using a lever arm, up until the point of maximum rotation, or until the component toppled over. The stage was then returned to its starting position, the component removed using tweezers (if it had not already toppled over), and the liquid removed from the binding site using a dry compressed inert gas. Liquid droplet volume was determined using the method described in section 3.2.7.

National Instruments LabView and Vision Builder AI software packages were used to create an inspection which tracked the component position relative to the binding site, and the angle of rotation of the stage. The two separate camera images were first transformed to greyscale to aid feature recognition. The fixed vertical edge of the rotating table was identified using straight edge detection to act as a datum plane, with the rotating portion of the stage tracked using a pattern matching algorithm. These were used to determine the angle of rotation of the stage which was overlaid to the image (Figure 3-14 a)). In the component image two straight edge detection algorithms were used to identify the horizontal edge of the binding site, and the vertical edge of the component. These were used to calculate the angle of the component relative to the binding site which was then overlaid onto the image (Figure 3-14 b)). Images from both cameras including overlays were recorded throughout the experimental procedure and data were logged to a spreadsheet. A list of the inspection steps is graphically summarised in a flowchart (Figure 3-15).

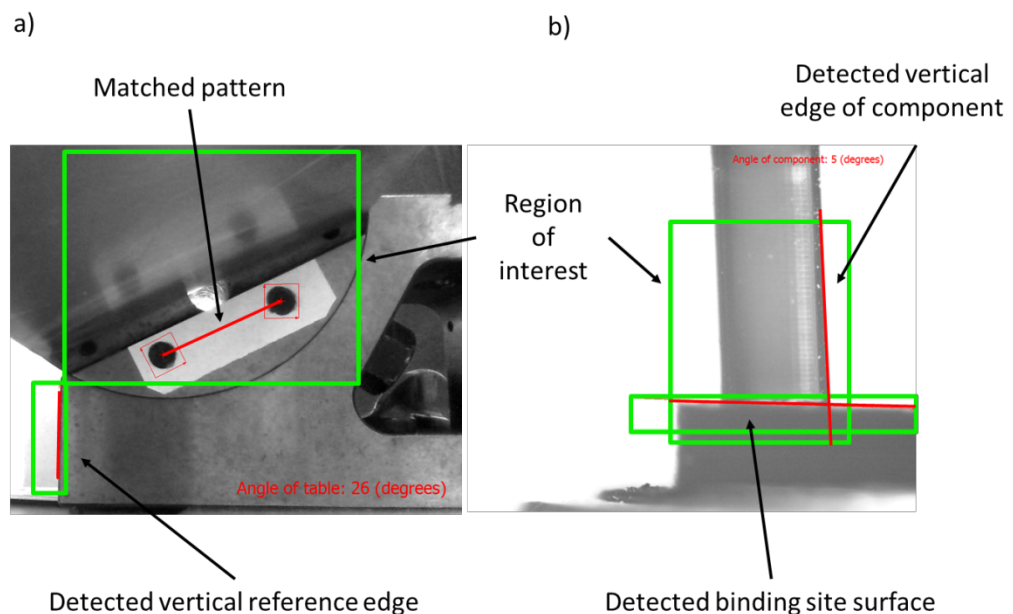


Figure 3-14: Inspection images from NI Vision for tipping experiments. a) tracking of table angle, b) measurement of component angle relative to binding site. Green boxes denote the regions of interest (ROI). Red lines show the algorithm detected features. Images enhanced for clarity.

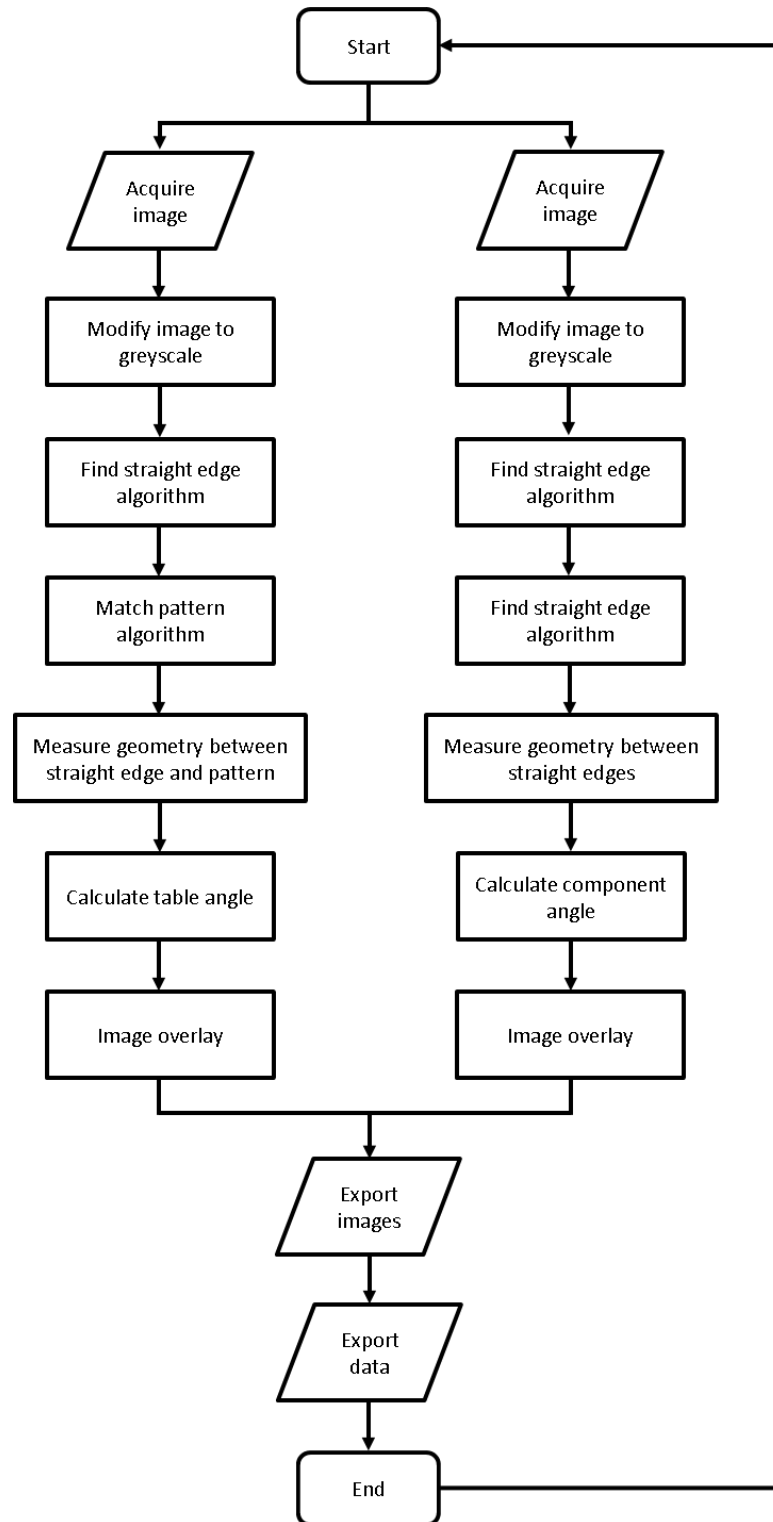


Figure 3-15: Flowchart of NI Vision inspection process for tipping experiments.

3.2.12 *Software tools*

In addition to the experimental activities, a number of software packages were utilised to realise the thesis. In the following subsection these programs are introduced and their use in the work identified.

ImageJ is a public domain, Java-based image processing program developed at the National Institutes of Health. ImageJ was designed with an open architecture that provides extensibility through user-created plug-ins and macros. Plug-ins have been developed by the community to achieve specific tasks and are also freely available in the public domain.

The LB-ADSA (Low Bond – Axisymmetric Drop Shape Analysis) plugin for ImageJ was developed by A.Stadler to measure the contact angle of low bond axisymmetric droplets. This was used to measure the contact angle of liquid water droplets placed on binding sites in chapter 5, section 5.1 of the thesis.

Minitab is a general-purpose statistical software package designed for easy interactive use. All graphing of data presented in this thesis was created using Minitab.

Surface Evolver is an iterative program that allows modelling of shapes determined by surface tension and other energies. A gradient decent method is used to evolve the system to a state of minimal surface energy, which can include surface tension, gravitational energy, squared mean curvature, user-defined integrals and knot energies, while subject to user-defined boundary conditions.

PTC Creo Parametric 2.0 is a commercially available CAD (Computer aided design) package that is widely used in industry. This software was used to design component test geometries and generate the STL files necessary for manufacture on the EnvisionTec Perfactory.

PTC Mechanism is a computer aided engineering (CAE) add-on package for Creo Parametric that allows forces and torques to be applied to model assemblies in order to conduct dynamic or static force analysis. This software was used to demonstrate the use of Surface Evolver derived spring constants in an industrially adopted design package (Chapter 8, section 8.2.3).

MATLAB is a widely used numerical computing environment and programming language developed by Mathworks. The software was used in the batch generation of data files for Surface Evolver, and in the extraction and processing of data from the simulations.

LabView, developed by National Instruments (NI), is a system design platform and development environment commonly used for data acquisition, instrument control and industrial automation. NI Vision software contains image processing algorithms and image acquisition functions that allow the development of complete machine vision applications. The software were used to develop a measurement strategy to visually track both the rotation of a stage and the angle of a component in real time and export the data in both numerical and graphical forms.

Testworks is a universal test software for the mechanical testing of materials, components, and finished goods. The software was used in conjunction with the Agilent G200 nanoindenter for the development and execution of the measurement strategy, as well as data acquisition.

3.3 Summary

In this chapter the major assumptions and limitations of the work carried out as part of the thesis were presented. The experimental procedures along with their technical limitations were detailed in section 3.2, Instruments and experimental procedures.

This chapter detailed the research methodology followed throughout the PhD project. In order to address the identified knowledge gaps a number of design

solutions for binding sites using the EnvisionTec Perfactory were proposed. A series of experiments were planned to examine the self-assembly of additively manufactured micro components using liquid surface tension. Surface Evolver, a free-to-use software package designed to model the shape of liquid surfaces shaped by surface tension was chosen to investigate a number of surface tension driven self-assembly conditions, and generate non-linear spring constants for individual DOF of component misalignment. Surface Evolver was also selected to model the non-idealised edge geometry of binding sites, typical of many manufacturing processes, and how these effect the alignment process. Finally the integration of the previously defined methodologies and models into a micro component test case is proposed and Surface Evolver derived spring constants integrated into a commercially available CAE package to illustrate the potential in an industrial design environment.

Chapter 4

4 ADDITIVE MANUFACTURE FOR MICRODROPLET ALIGNMENT

This chapter introduces the use of an additive manufacturing process for the fabrication of structures intended for microdroplet self-alignment applications. The equipment used was an EnvisionTec Perfactory Mini-Multi lens projection micro stereolithography machine using EnvisionTec R11 rapid prototyping material. It is a layer-based manufacturing method that utilises the controlled solidification of a light sensitive liquid polymer (photopolymerisation) to generate complex 3-dimensional structures.

One of the advantages of the manufacturing technique (and other additive manufacturing techniques in general) is that they offer very short lead times from the design phase through to fabrication. The manufacturing process is highly flexible, and does not require special tooling for specific jobs as is associated with traditional subtractive manufacturing processes. The manufacturing technique is particularly attractive for microdroplet component alignment as it allows the integration of special features (binding sites) for liquid containment into the component at no additional manufacturing cost. This is compared to other techniques for binding site generation which rely on additional machining operations, or chemical treatment to create contrasts in wettability in order to influence liquid droplet behaviour.

This chapter introduces the concept of additively manufactured structures for use in microdroplet alignment applications. It outlines the rationale for the research approach undertaken and presents the process that was followed in developing procedures and designs suitable for microdroplet alignment. All components were manufactured using the EnvisionTec Perfactory Mini-Multi lens projection stereolithography machine at the University of Nottingham, and as such the conclusions drawn may not be applicable to other AM processes. The chapter begins by looking at the design of components on the Perfactory for microdroplet alignment and discusses some of the inherent limitations of the system. A number of the design rules presented are specific to the project

objectives such as the arraying of binding sites (section 4.2.2), channels for liquid transfer (section 4.2.7), patterning of hydrophobic features (section 4.2.8), while others are more generic and could be applied to the manufacture of other types of component on the Perfactory. The chapter then considers manufactured component quality and looks at the occurrence of defects in the additively manufactured structures and techniques which can be employed to either limit or prevent them.

4.1 Functional binding sites by additive manufacture

The containment of the liquid droplet to the binding site is of key importance to the assembly process. The assembly process relies on the minimisation of the surface energy of the liquid droplet which occurs when the component and binding site (which have the same shaped surface in contact with the liquid) are well aligned with one another. If the liquid droplet is able to overflow the binding site the component will be drawn along with the liquid and misalignment will occur.

The literature has shown that the use of binding sites for microdroplet alignment is an effective technique for the self-assembly of micro components. The literature has mainly focused on the application of microdroplet alignment for integrated circuit (IC) dies onto silicon wafers. Binding sites for these applications have been created by growing an oxide layer on the silicon wafer surface, followed by a patterning and reactive-ion etching process. To date there has been no investigation into the manufacture of binding sites for microdroplet alignment using additive manufacturing techniques. To examine the capability of AM structures for microdroplet alignment a number of key aspects needed be investigated. Firstly the process must be capable of fabricating precise geometric features. These are necessary as the alignment of the component relies on the containment of the liquid droplet to the binding site surface. Two geometric shapes were investigated in this thesis: circular binding sites for the investigation of liquid containment on the binding site, and square binding sites for the self-assembly of micro components. Different designs were investigated for structures with internal channels to move liquid

from a central reservoir to the binding site via capillary action. Patterned geometric features were examined to establish if these were suitable to create hydrophobic regions on the component. Additionally the use of undercut binding sites was investigated in order to offer a more robust containment of the liquid droplet based on the Gibbs inequality.

4.2 Characteristics of the EnvisionTec Perfactory

4.2.1 *Basic operation*

The working envelope for parts produced on the EnvisionTec Perfactory is 12 x 14 x 230 mm in x, y and z-axes respectively. This area can be used to produce a single component, or multiple components that fit within the prescribed footprint.

The EnvisionTec Perfactory is a layer-based additive manufacturing process that builds components through a controlled solidification of a liquid, light-sensitive resin when exposed to a light source. As each layer is cured the build plate moves upwards in the z-direction. The build time for components is determined by the time to cure each successive layer, rather than the complexity, or x-y dimensions of the part. This means that increasing the z-height of a component significantly increases the build time, and is therefore an important factor to be considered in the design of components. The build time is constant throughout the build process and is able to realise 10 mm/hr at a layer thickness of 50 μm [180]. The layer thickness, which is also referred to as the dynamic voxel thickness (Z), is determined by the type of resin used and is set within the Perfactory RP software. All components manufactured in this thesis were produced using EnvisionTec R11 rapid prototyping material which has a minimum layer thickness of 25 μm .

4.2.2 *Manufacturing of components in test array*

Test structures were designed in an array to maximise the number of features that could be produced on each component, limiting both material usage and manufacturing time. The components housing the test arrays were 10 x 12 x 2

mm (in x, y, and z axes respectively) to provide a size that was both robust and easy to handle, while complying with the maximum build envelope of the Perfactory system. Consideration had to be taken to ensure there was sufficient space between features to promote removal of any uncured and excess resin during the cleaning stages. It was also important to allow appropriate clearance between the features of interest and the surrounding bulk material, in order to prevent any overflow of the liquid droplet during alignment applications that may span both regions, thus affecting the assembly process.

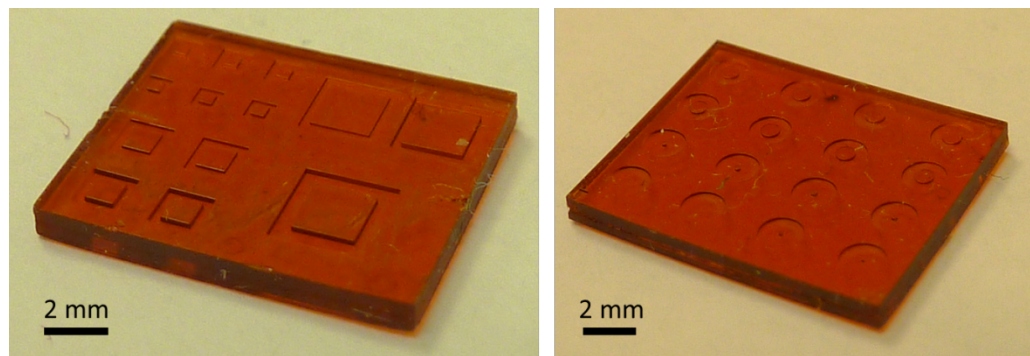


Figure 4-1: Binding sites arranged in test array. (left) range of square binding sites, (right) range of circular binding sites.

4.2.3 *Minimum size of features*

Although the machine specification for the minimum voxel size was stated earlier, it was still unclear as to the minimum size of free-standing structures that could be reliably reproduced. In order to determine this, a number of square and circular binding sites were manufactured in test arrays with dimensions from 5 mm down to 50 μm . An example test array can be seen in Figure 4-2 which featured binding site dimensions from 50-300 μm , in 25 μm increments. The array featured 11 sizes for both square and circular designs, with 4 repeats for each size, resulting in a total of 88 binding sites on the array.

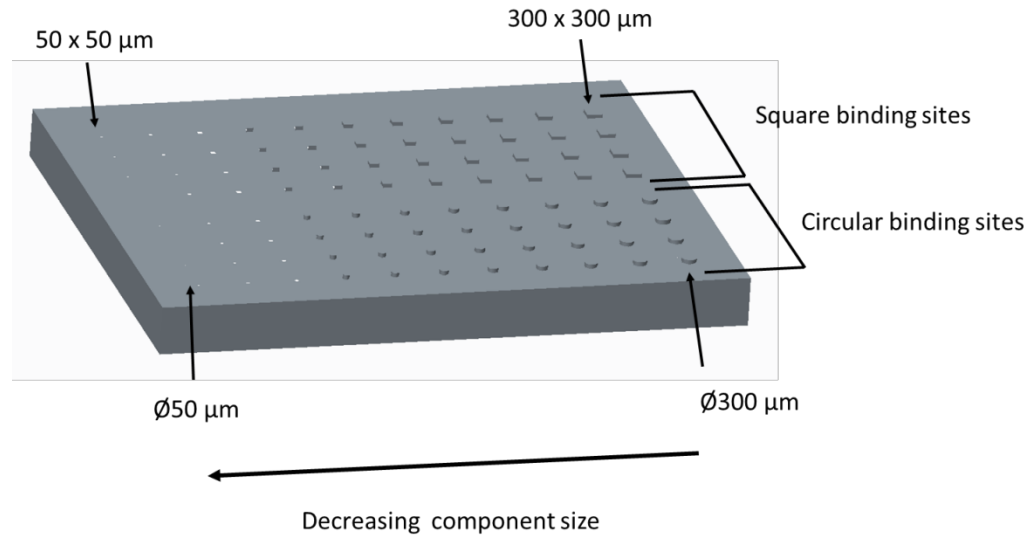


Figure 4-2: Rendered CAD image of test array containing square and circular binding sites. Dimensions of binding sites from 50 - 300 μm , in 25 μm increments.

Components were inspected using optical microscopy for conformity and presence of defects. It was found that the smallest free-standing features that could be reliably produced were $\text{Ø}200\text{ }\mu\text{m}$ circles, and $200 \times 200\text{ }\mu\text{m}$ squares. Below this size the features were unable to be reliably resolved, resulting in incomplete or poorly defined features.

4.2.4 *Minimum layer thickness*

As previously discussed the EnvisionTec Perfactory is a layer-based manufacturing method. In order to increase the resolution of components produced on this machine it is desirable to have the smallest layer thickness possible. Using the EnvisionTec R11 resin a layer thickness of 25 μm is able to be realised, as opposed to the R5 resin which has a minimum layer thickness of 50 μm (Figure 4-3). The minimum layer thickness for supported resins can be found within the Perfactory RP software.

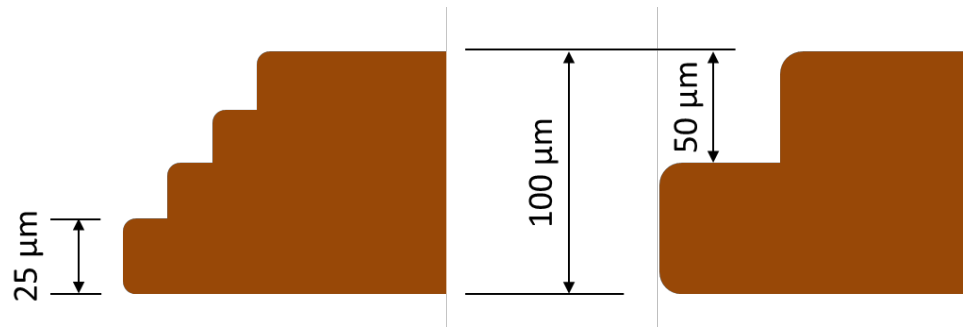


Figure 4-3: Diagram illustrating the effect of layer thickness on component resolution for a 100 μm high structure. Left is for 25 μm layer thickness, with 50 μm layer thickness displayed on the right.

The design of the binding sites for liquid self-assembly is important as they must have a sufficient number of layers in order to recreate the desired geometry. It is also desirable to limit the number of layers to keep the profile of the structure low so as not to interfere with the overall form or function of the component design. An additional consideration is also the trade-off between increased resolution (more layers), and the risk of defects occurring in a given layer.

It was decided that an overall binding site height of 100 μm was sufficient to reproduce the sidewall geometry, while keeping the profile suitably low. This resulted in a thickness of 4 build layers in the z-direction.

4.2.5 *Support structures*

In order to aid in the manufacture of the components, any feature that has a significant overhang will require a support structure to be added. This is required to prevent the feature from collapsing under its own weight as the build plate moves. Support structures are also necessary to allow the component to be removed from the base burn-in layer. Support structures are typically circular based columns 0.4 - 0.6mm in diameter. They can be easily removed by cutting through them using a scalpel. A Schematic of a typical component manufactured on the Perfactory containing support structures can be seen in Figure 4-4.

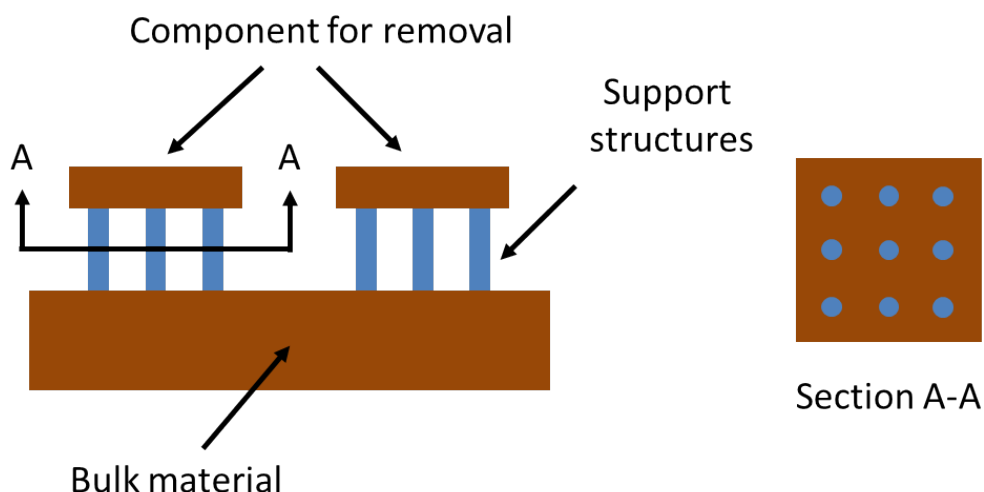


Figure 4-4: Schematic showing typical component manufactured on the Perfactory, utilising support structures. Support structures indicated in blue for clarity..

It is recommended that the support structures be equally spaced to offer maximum support to the overhanging component. Sufficient clearance must be left between successive supports to readily allow the removal of excess resin during the post-build cleaning process.

It is important to consider the placement of the support structures and also the orientation of the component during the build process. The integrity of the faces used for the assembly process are of the utmost importance as the occurrence of any defects or damage is detrimental to the self-assembly process. This means that support structures cannot be placed on these faces. It is also recommended that the assembly faces are normal to the build direction to ensure a flat, even surface is produced. This means that components used in the assembly process will typically need to be designed upside-down so the binding site face is upward facing.

4.2.6 *Fabrication of binding site geometries*

The structures considered for this work were simple geometric shapes of squares and circles. Circles were chosen with the intention to examine the ability to pin isolated water droplets. When placed on a flat surface an unconstrained liquid droplet will adopt a circular profile at the liquid-solid

interface, as this is its lowest energy state. A circular binding site was considered suitable to examine the structures ability to pin the liquid without forcing the droplet to wet to an intricately shaped surface which would distort the droplet shape.

Square binding sites were chosen as these are able to offer both lateral and rotational alignment when carrying out self-assembly processes using liquid surface tension. For this to occur, the binding site and component must have the same shape in contact with the assembly liquid. The component then moves on the liquid film until it reaches its lowest energy state. This is when the component and binding site are well aligned.

4.2.7 *Channels for liquid transfer*

Consideration was given to the application and transfer of the assembly liquid to the binding site. A number of different designs were attempted in order to draw the assembly liquid from a central reservoir, with internal channels taking the liquid to the binding site. In practise however these were found to be unsuccessful as the internal channels were unable to be manufactured correctly and were blocked with semi-cured resin, thus preventing the transfer of liquid via capillary rise through the channel.

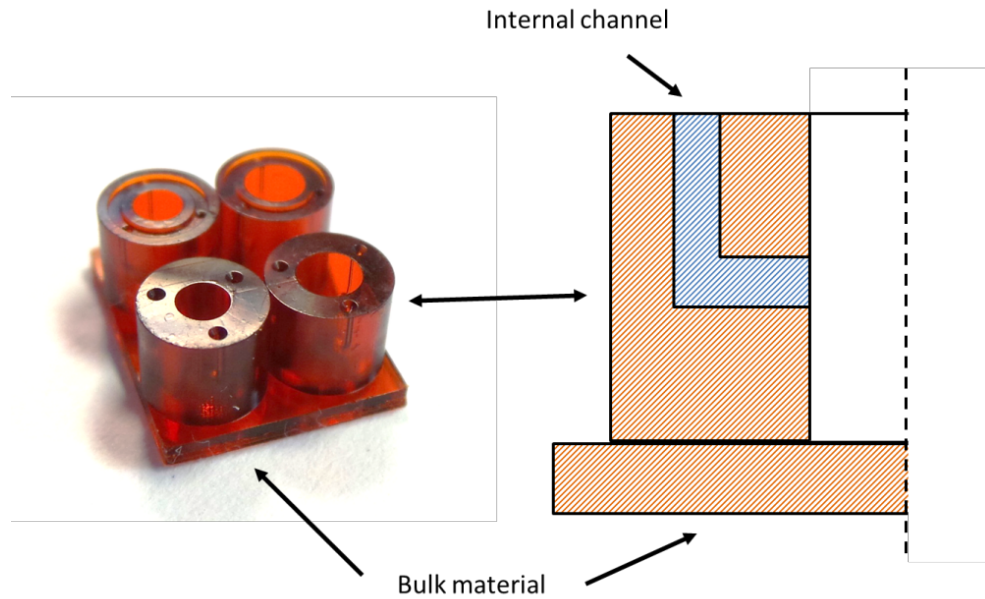


Figure 4-5: (Left) Example test array featuring internal channels produced on the EnvisionTec Perfactory. (Right) Cross-sectional diagram showing the internal channels in the component.

4.2.8 *Patterned surfaces to create hydrophobic regions*

The alternative method to pinning the triple contact line (TCL) at a geometric edge in order to control the spreading of a liquid is to create a difference in wettability between certain regions of the component. By surrounding the binding site with a hydrophobic surface the liquid can be encouraged to wet the more hydrophilic region and thus control where the liquid sits. This can be achieved through a chemical process to alter the material properties, or by patterning of micro-pillar arrays similar to those seen in nature. The work presented in this thesis is concerned with the investigation of additively manufactured binding sites which can be created in one step, and do not require any additional processing. Therefore only the use of micro-pillar arrays to create hydrophobic regions was considered in this work. Experimental investigation of the micro-pillar arrays found that these were unable to be realised using the EnvisionTec Factory. The feature sizes able to be produced on the Perfactory were not small enough to be able to achieve a contrast in wettability between the main binding site surface and the surrounding micro-pillar array.

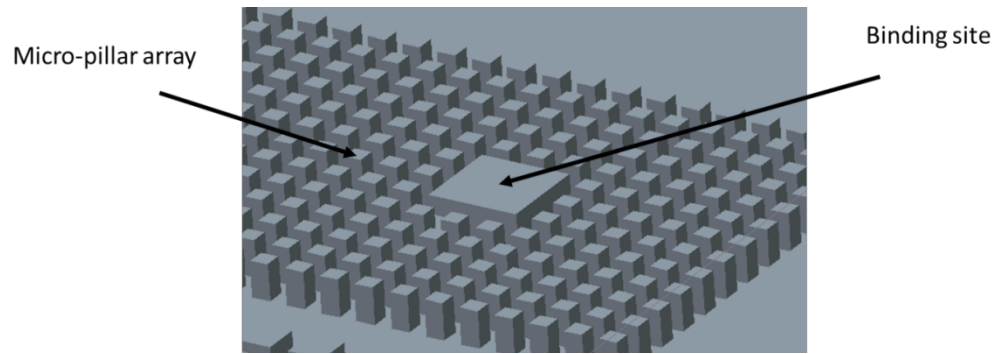


Figure 4-6: Rendered image of binding site surrounded by a micro-pillar array.

4.2.9 *Edge geometries*

The binding sites investigated in this thesis do not contain any chemical treatment to create a contrast in wettability between the binding site and bulk material. The binding sites utilise a physical edge to halt the movement of the liquid droplet, with the maximum achievable contact angle determined by the Gibbs inequality (see chapter 2, section 2.4.12). Droplet motion is halted at the physical edge due to the triple contact line becoming pinned to the geometry, much in the same way as the phenomenon of contact angle hysteresis introduced in Chapter 2, section 2.4.10 occurs. The physical edge creates a significant energy penalty which must be overcome for droplet motion to continue down the binding site sidewall. This energy penalty means it is therefore preferential for the liquid droplet to remain pinned to the binding site. This pinning condition remains valid as long as the contact angle between the liquid droplet and binding site does not exceed the maximum contact angle described by the Gibbs inequality. Once the contact angle is exceeded the droplet is able to flow over the physical edge and is no longer constrained to the designated binding site area.

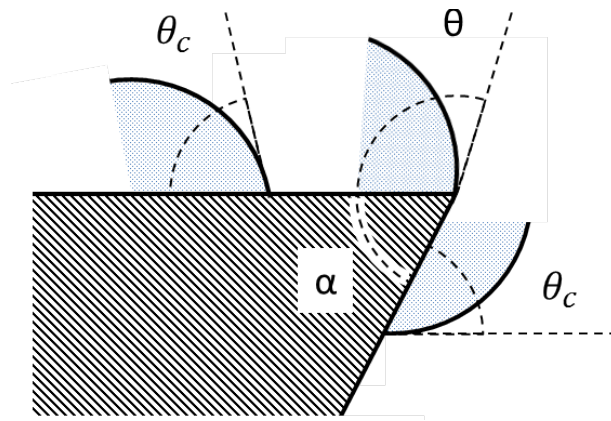


Figure 4-7: Spreading of a liquid droplet meeting a sharp edge as described by the Gibbs inequality, equation (2-14). Figure reproduced from chapter 2, section 2.4.12.

Undercutting the binding site geometry allows the contact angle to be significantly increased over that of the static contact angle on a plain flat surface. An increase in contact angle means the droplet is able to undergo more deformation in shape (bulging over the binding site) before overflowing the binding site top surface. This means the assembly process will be tolerant of more severe initial component misalignments, or increased component mass, without the risk of liquid overflow.

A detailed investigation of the ability of the EnvisionTec Perfactory to fabricate the undercut features is presented in chapter 5, section 5.2.

4.3 Component quality

As previously mentioned, self-assembly of components using liquid surface tension relies on the containment of the assembly liquid within a specified region. If the integrity of this region is compromised through manufacturing defects or mechanical damage the liquid is able to flow into undesirable positions which have a detrimental effect on the alignment process. Examples of typical defects encountered during the manufacture of components by the author can be seen in Figure 4-8. A detailed analysis of the types of common defect, their influence and how to avoid or minimise them will be presented in the following sub-sections.

As component size is decreased the occurrence of any defects in the structure has a greater impact on the assembly performance. Conversely as components become larger the effect of any one defect becomes less significant, however due to the increased perimeter the risk of defects occurring becomes higher. It therefore becomes apparent that steps should be taken to ensure the integrity of the components, particularly the edges, if accurate and repeatable self-alignment is to be achieved.

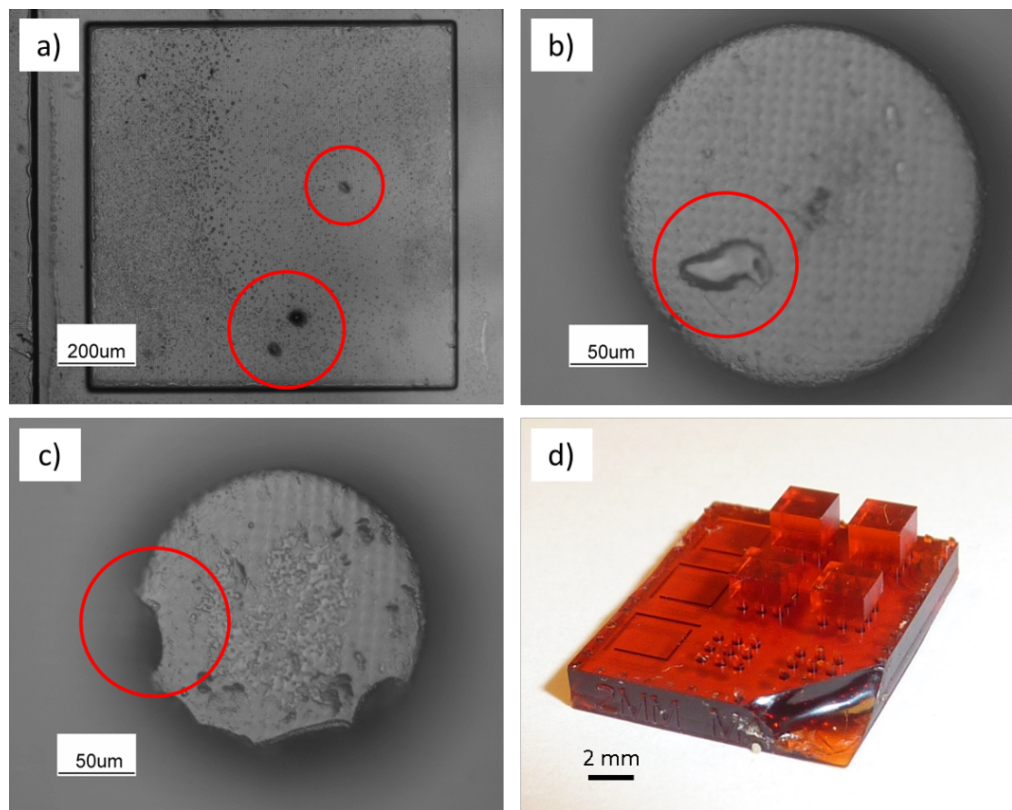


Figure 4-8: Images of generic defects encountered during manufacture on the EnvisionTec Perfactory. Defects have been highlighted in red. a) Pit marks in the surface, b) inclusion of foreign material, c) brittle failure of component edge, d) brittle failure caused during removal from build plate.

4.3.1 *Protection of binding sites*

The containment of the assembly liquid within the designated binding site is crucial to the success of any assembly operations using liquid surface tension.

It is therefore clear that steps should be taken to ensure the integrity of the binding site during any handling operations. This includes all stages from the end of the manufacturing process, where the component must be removed from the build plate and cleaned, through to testing and implementation where liquid must be deposited on the binding site, and the component placed.

As previously mentioned (section 4.2.2) the bulk of the test array was designed to be close to the maximum dimensions for the Perfactory, with the part being 10 x 12 mm in order to provide a robust unit that was easy to handle. The thickness of the bulk material was chosen to be 2 mm to allow easy removal from the EnvisionTec Perfactory build plate without risk of mechanical damage or warping.

The first set of structures which were manufactured had the features proud of the bulk material surface as shown in Figure 4-9.

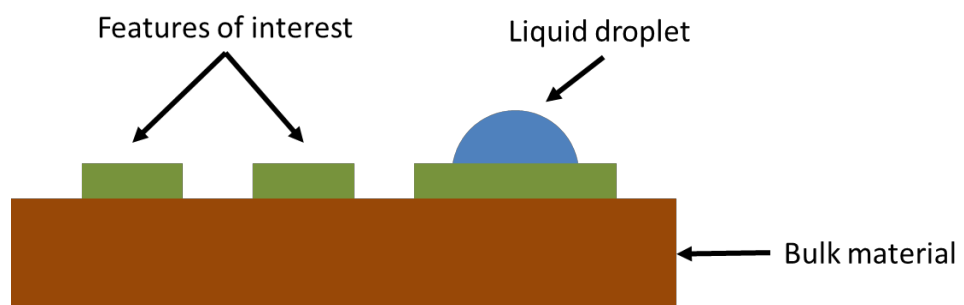


Figure 4-9: Diagram illustrating the features sitting proud of the bulk material surface. Features have been shown in green with example of liquid droplet placement shown for clarity.

Examination of the components under optical microscopy showed that binding sites were very susceptible to mechanical damage during the removal and cleaning phases. As previously mentioned the component is removed from the Perfactory glass build plate by sliding a scalpel blade underneath it. The component is then handled using a pair of tweezers. Components are cleaned by submerging in a glass beaker of isopropanol alcohol, and then placing the beaker in an ultrasonic bath. Components are then removed from the alcohol using a pair of tweezers and allowed to air dry. During these handling and

cleaning operations there are multiple opportunities for mechanical contact with the features of interest if they are sitting proud of the bulk material surface. This led to parts of the binding site being damaged due to brittle failure (Figure 4-10).

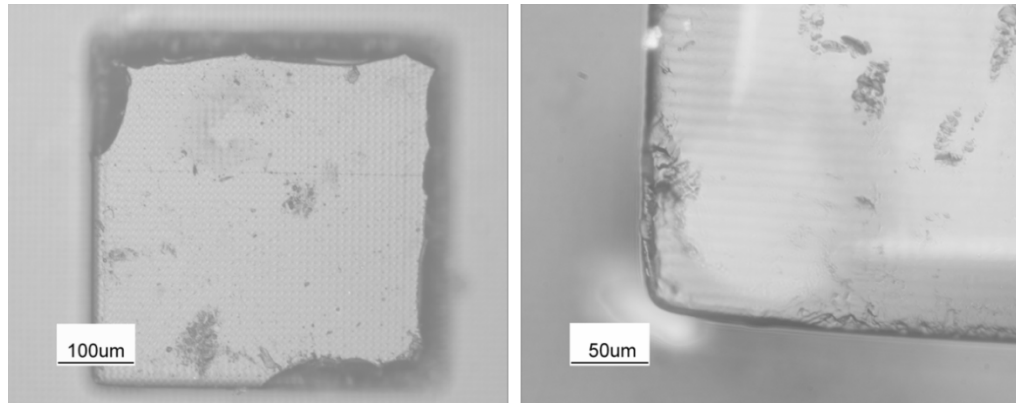


Figure 4-10: Optical microscope images of damaged square binding sites sitting proud of the bulk material surface. Binding site dimensions are 0.5 x 0.5 x 0.1 mm.

In order to combat this, binding sites were redesigned to have their top surface sitting flush with the bulk material, with the necessary four layers height achieved by surrounding them with a “trench”, 100 µm deep. A cross-sectional diagram of the concept is shown in Figure 4-11.

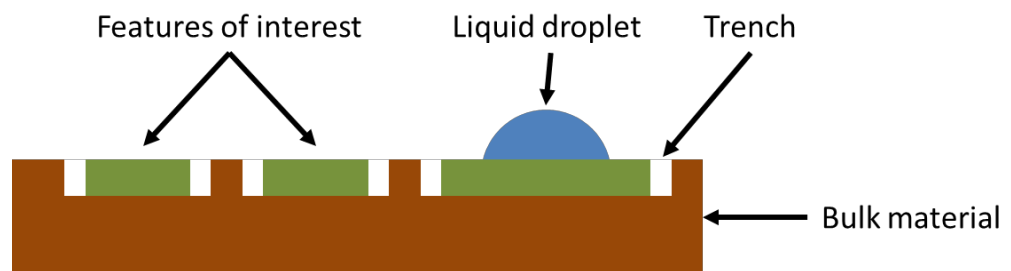


Figure 4-11: Cross-sectional diagram showing the binding sites surrounded by a trench, keeping the features of interest flush with the bulk material surface. Features of interest are displayed in green with example of liquid droplet placement shown for clarity.

Components were manufactured and cleaned using the aforementioned process and examined using optical microscopy (Figure 4-12). This method of protecting the binding site with a surrounding trench, keeping the top surface

flush with the bulk material, offered a much more reliable yield rate. Binding site edges were much less susceptible to mechanical damage and thus reduced the likelihood of any defect occurring which would be detrimental to the structures ability to pin the assembly liquid's TCL, thus hindering the self-alignment process.

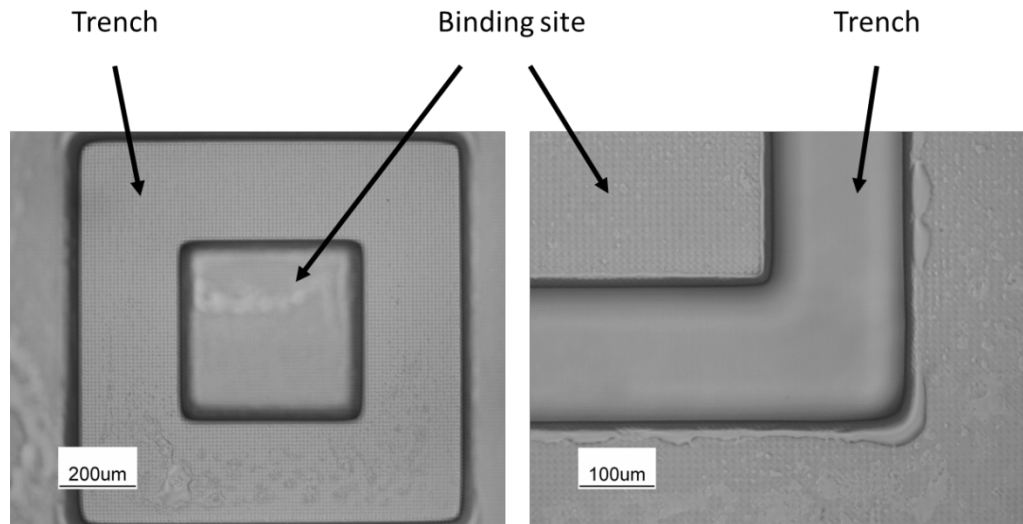


Figure 4-12: Optical microscope images of component with recessed features. (Left) binding site dimensions 0.5 x 0.5 x 0.1 mm, (right) binding site dimensions 1 x 1 x 0.1 mm.

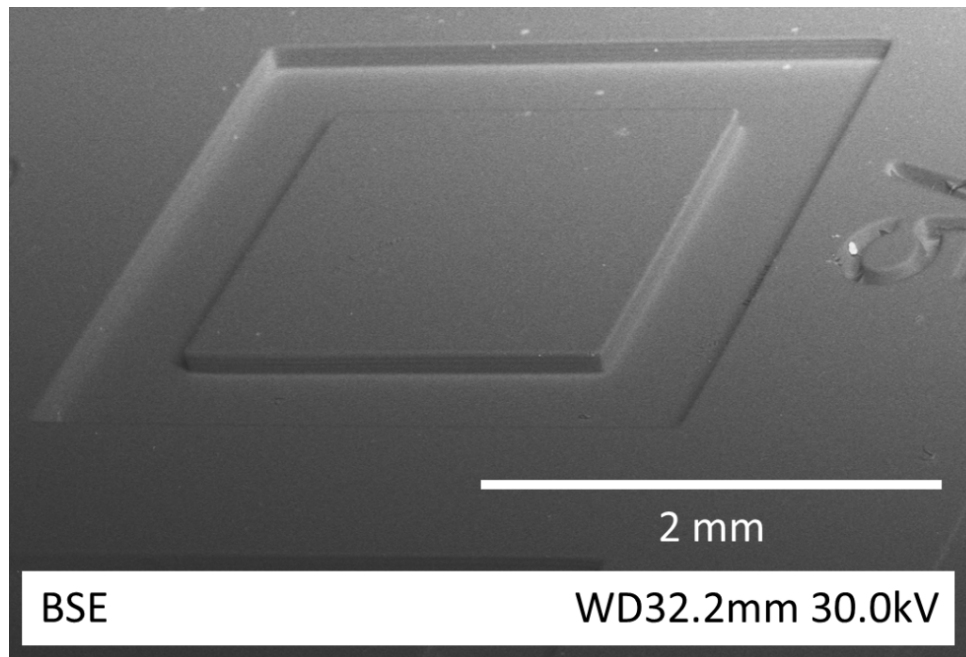


Figure 4-13: SEM image of test array containing a 2 x 2 x 0.1 mm binding site with 75° edge geometry.

4.3.2 *Protecting the surface of binding sites and components*

The self-assembly tasks were planned to be carried out using components that were also additively manufactured using the EnvisionTec Perfactory. These components needed to be manufactured using support structures in order to allow them to be removed from the base-plate following the cleaning operations. This resulted in components that were therefore sitting proud of the bulk material and needed to be protected in some way to avoid damage occurring during the handling and cleaning operations.

First the test array was given a series of 8 short posts that were taller than the components that needed protecting (Figure 4-14). These were found to not offer adequate protection as the components could still be accidentally damaged during the handling operation when using the tweezers.

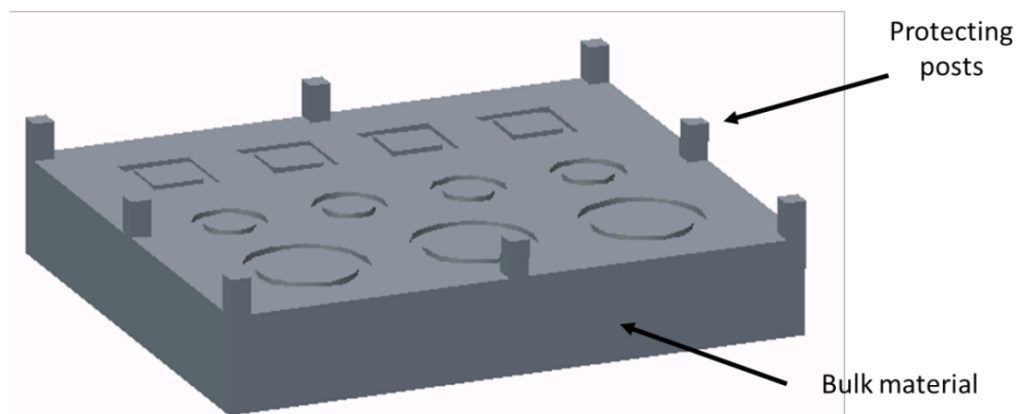


Figure 4-14: Rendered image of test array featuring protecting posts

The chosen design was a retaining wall that went around the perimeter of the components that sat on its own support structures (Figure 4-15). This wall was then removed post cleaning operation by cutting through the supports using a scalpel blade and discarded.

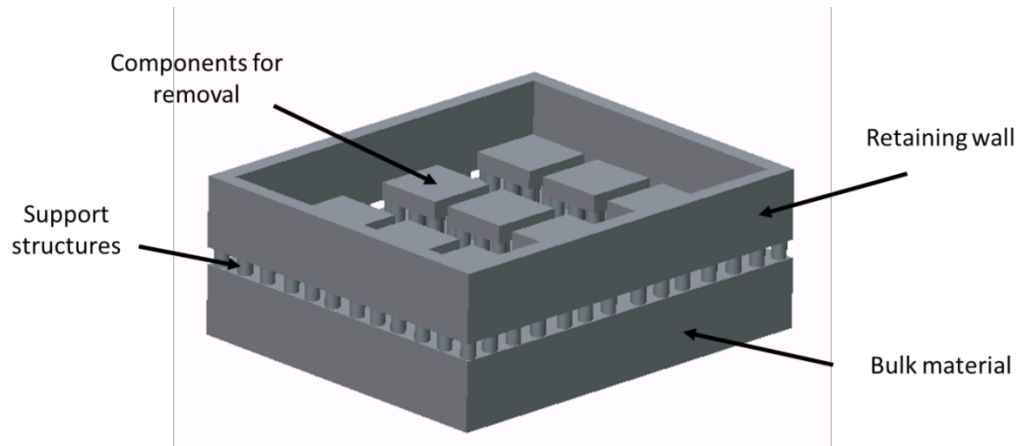


Figure 4-15: Rendered image of test array surrounded by protective retaining wall

This design was found to offer a much higher yield rate of components that were free of significant defects caused by mechanical damage. An example of a series of components in test arrays before and after the removal of the retaining wall can be seen in Figure 4-16.

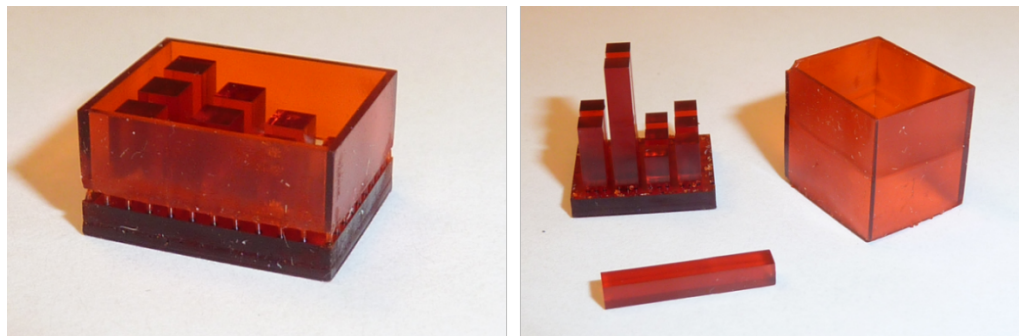


Figure 4-16: Examples of test arrays surrounded by retaining walls. (left) before removal of retaining wall, (right) after removal of retaining wall showing components still on array, alongside removed component and wall.

4.4 Summary

In this chapter a set of design rules have been established for the fabrication of additively manufactured micro components for microdroplet alignment. A number of considerations were taken into account such as feature size and shape, layer thickness, use of support structures, transportation of liquid, hydrophobic regions, and undercut structures. Additionally guidelines for how to minimise or prevent damage to components and features are presented.

Binding sites were manufactured on test arrays of dimensions 10 x 12 x 2 mm. Circular and square binding sites of dimensions ranging from 5mm - 50 μm were investigated to establish the smallest size that could be reliably produced. It was found that circular sites of $\varnothing 200 \mu\text{m}$ and square sites of 200 x 200 μm were the smallest features that could be resolved. A binding site height of 100 μm (4 build layers) was selected to offer sufficient number of layers to realise the geometry, while also being small enough to not impact on the overall component design.

Design rules were presented for the use of support structures with components for microdroplet alignment. It was suggested that binding sites, and assembly faces of components be upward facing and free from support structures. This is driven by the need for a flat, uniform and defect free surface for the assembly process.

One of the disadvantages of the manufacturing technique is that the components are susceptible to mechanical damage. In order to minimise the risk of damage, important features such as the binding site were surrounded by a trench in order to keep them flush with the surrounding bulk material of the component. This was done to protect the edges of the binding sites which are of key importance in constraining the flow of liquid droplets. In order to protect components intended for assembly tasks the array was surrounded with a protecting wall which could be cut away after post-build cleaning was completed. Both of these techniques offered significant improvements in the yield rate of binding sites and components which were free from defects and suitable for experimental investigation.

A great deal of time and effort was expended in the practical pursuit of high quality and repeatable AM structures for microdroplet alignment. With these procedures in place and large number of components produced, it was possible to conduct experimental investigations into binding site performance. At this stage the effectiveness of the structures for microdroplet alignment applications has yet to be determined. In the following chapter an experimental

investigation of the structures ability to control liquid droplet spreading is introduced. Cross-sectional analysis of the binding sites is carried out to assess the manufacturing processes ability to reproduce the desired geometry. Finally a series of challenging self-assembly experiments are performed to evaluate the ability of the binding sites to offer accurate and repeatable alignment of components.

Chapter 5

5 EXPERIMENTAL INVESTIGATION OF MICRODROPLET COMPONENT ALIGNMENT

One of the key requirements in liquid self-assembly is the confinement of the assembly liquid to a designated area. This area is typically referred to as the binding site. Flow of the assembly medium outside this area is catastrophic and leads to uncontrollable alignment of the component. As described in chapter 2, section 2.3.1 there are a number of methods that have been used to create binding sites which can be divided into two distinct areas: those which alter the surface properties of the material to create a contrast in wettability [26, 68-72]; and those that rely on a secondary process to create well-defined sharp edges [78-81]. This chapter investigates the use of purely topographical structures that have had no further surface modification techniques applied to them in order to influence wetting properties. In addition, the structures are created using a flexible, additive manufacturing process that is able to generate both the component of interest and the binding site in a single process step.

A range of different sized binding sites and edge geometries are examined and their ability to support isolated liquid water droplets is presented and their contact angle measured. Cross-sectional analysis of the test structures is presented to establish the ability of the additive manufacturing process to realise suitable edge geometries. The ability of the binding sites to offer precision alignment through self-assembly is experimentally investigated through three challenging assembly conditions. The assembly conditions presented are that of lateral, rotational, and combined lateral component misalignment. Finally an investigation of liquid droplet behaviour on binding sites is experimentally investigated through a novel application of a nanoindenter machine.

5.1 Constraint of liquid spreading using topographical structures

The natural contact angle for water on the polymer material used in this work was previously determined in chapter 3, section 3.2.6. The experimental measurements found the contact angle to be 70° with a standard deviation of

3°. Optical microscope images illustrating the difference between the natural contact angle on the plain substrate and an isometric view for an undercut binding site can be seen in Figure 5-1. These illustrate the dramatic effect on the droplet size and shape that is made possible with the undercut binding sites.

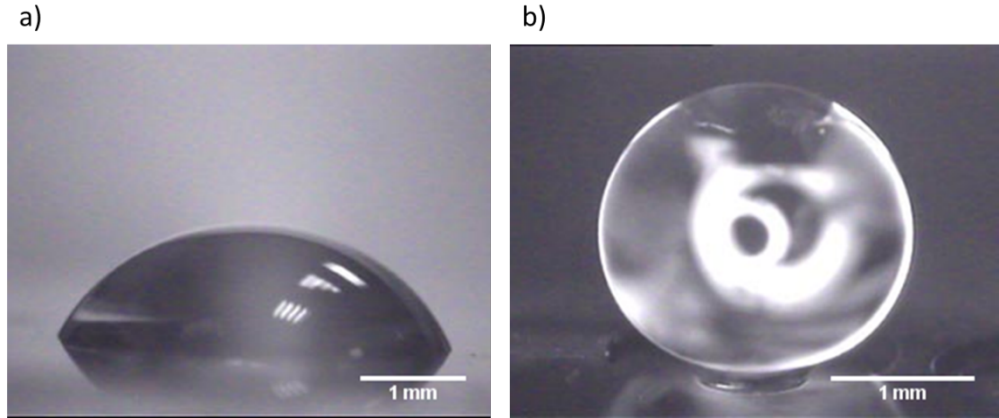


Figure 5-1: Optical microscope images of water droplets; a) unconstrained droplet on plain substrate, b) isometric view of droplet constrained to Ø1 mm circular binding site with an undercut 60° nominal edge geometry.

The results collected for the maximum contact angle before droplet collapse are shown in Figure 5-2, plotted against nominal edge geometry. Each data point represents an average of 10 measurements, with error bars displaying standard deviation. From these data it can be seen that higher contact angles were achieved for the Ø0.5 mm binding site compared to the Ø1 mm site. There are a number of reasons that could explain this result: firstly by doubling the diameter of the binding site the surface area is increased by a factor of 4. This would mean that the binding site surface is able to hold a significantly greater volume of liquid. When the droplet is small enough gravitational effects will be negligible but as the diameter approaches a certain length, known as the capillary length (equation (5-1)), they will start to play a role once again. For water at atmospheric pressure and 20° Celsius: $\gamma = 72.8 \text{ mN m}^{-1}$, $\rho = 998.21 \text{ kg m}^{-3}$, $g = 9.81 \text{ ms}^{-2}$, giving a capillary length of 2.7 mm.

$$\lambda_c = \sqrt{\frac{\gamma}{\rho g}} \quad (5-1)$$

Where, g is acceleration due to gravity, ρ is fluid density and γ is surface tension. The average measurement of the droplet diameter for the binding site achieving the highest contact angle on the Ø0.5 mm binding site was 1.32 mm, whereas for the Ø1 mm site an average diameter of 2.12 mm was measured. This shows that for the larger diameter binding site the droplet diameter had started to approach the capillary length, leading to gravitational effects acting on the droplet with proportionally greater effect. It is therefore proposed that this could have the effect of making the droplet unstable, causing it to collapse at lower contact angles.

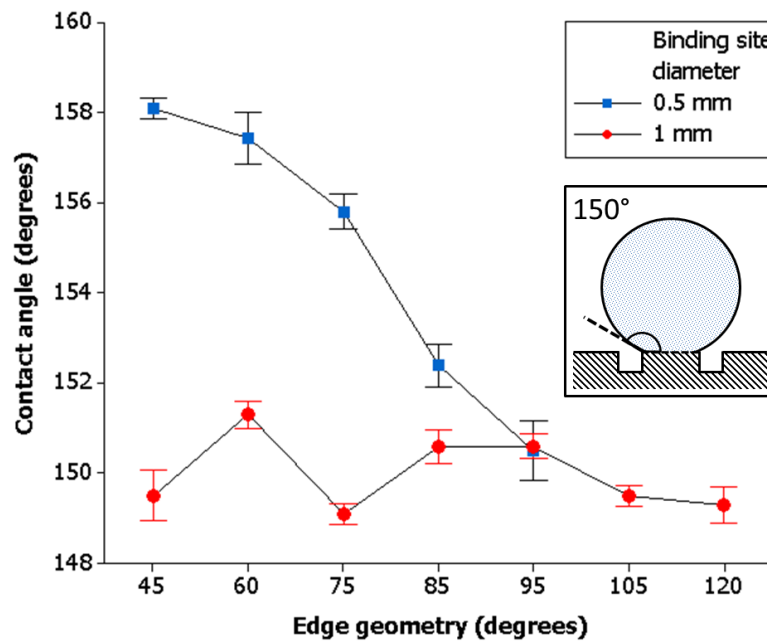


Figure 5-2: Contact angle of water droplets on circular binding sites for full range of nominal edge geometries. Error bars display standard deviation.

Other factors that could influence a lower contact angle are also any defects that occur on the edge of the geometry. As the diameter of the structure increases, so too does its perimeter, and with a greater perimeter length the likelihood of manufacturing defects along the length of this critical feature

increases. Preventing liquid spreading with a topographical edge relies on the integrity of the structure. Once the droplet begins to slide down the vertical face of the structure failure is uncontrollable and catastrophic, leading to droplet collapse and spreading outside of the designated binding site. This type of droplet behaviour is therefore undesirable for self-assembly applications. The data also shows that contact angles decrease rapidly for Ø0.5 mm binding sites once the edge geometry becomes larger than 75°. It should be noted that no data was plotted for 105 -135° for Ø0.5 mm, and also 135° for Ø1 mm. This was due to the fact that as the angle increased above 105° the binding sites were not able to support the liquid droplets with good stability. As a result the droplet would slide down the vertical face almost immediately, becoming pinned once the bottom of the slope had been reached. Although the volume of the droplet was able to be increased when in this position and did not immediately collapse, the fact that it was no longer constrained to the binding site was deemed unacceptable as this would cause systematic misalignment during self-assembly of a component. Based on the initial findings, only edge geometries from 45-90° were examined for the remainder of the binding site diameters. Data presented in Figure 5-3 show fairly close grouping as there is only a difference in contact angle of 9° across all binding sites. Points of interest from this graph are the low contact angle measured for Ø0.6 mm x 45°, and the missing data point for Ø0.4 mm x 45°.

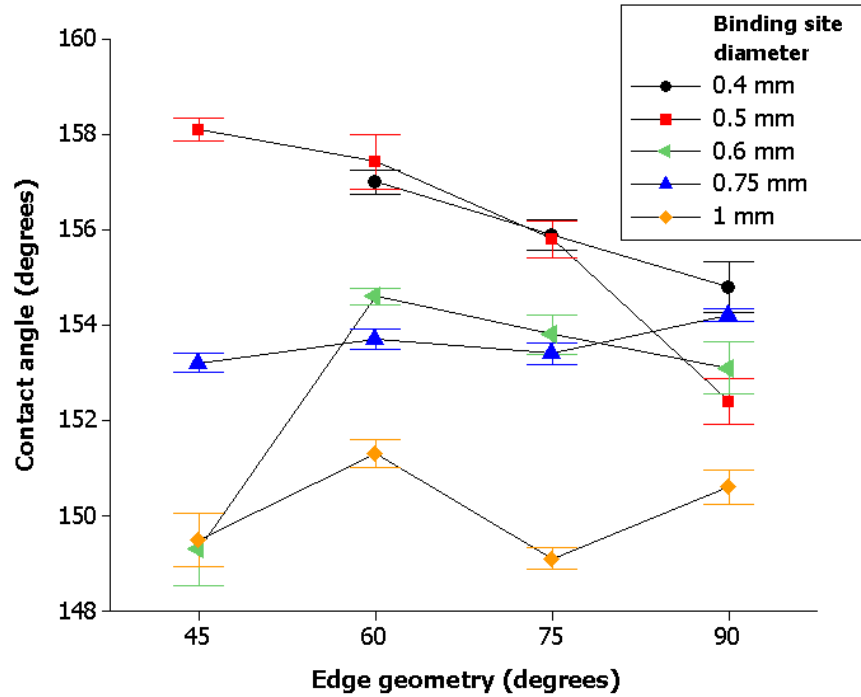


Figure 5-3: Contact angle of water droplets on circular binding sites for different nominal edge geometries. Error bars display standard deviation.

In order to investigate the cause of the missing data points subsequent SEM analysis of these binding sites was performed. This revealed from analysis of their geometry that these particular structures were either damaged in the manufacturing process or failed to build correctly. Figure 5-4 a) and b) show Ø0.4 mm binding sites, and c) and d) show Ø0.6 mm binding sites. Both images a) and c) appear to have a jagged edge which would indicate a brittle failure which could have been caused by mechanical damage to the structures. Image d) appears to be smoother and would point towards a defect in the build process. The top surface of the structure in image b) can be seen to be curling upwards which would suggest a contraction of the resin due to evaporation. This contraction of the partly cured resin has led to the development of cracks in the structure which are indicated in the image by white arrows. It is worth noting that none of these manufactured structures visibly displayed a 45° edge geometry and would imply that this level of negative incline (1:1) may not be suitable for the manufacturing method. However, it can be seen from Figure 5-2 and Figure 5-3 that for binding sites with a diameter of 0.5 mm or less there is a practical benefit to using edge geometries below 90°.

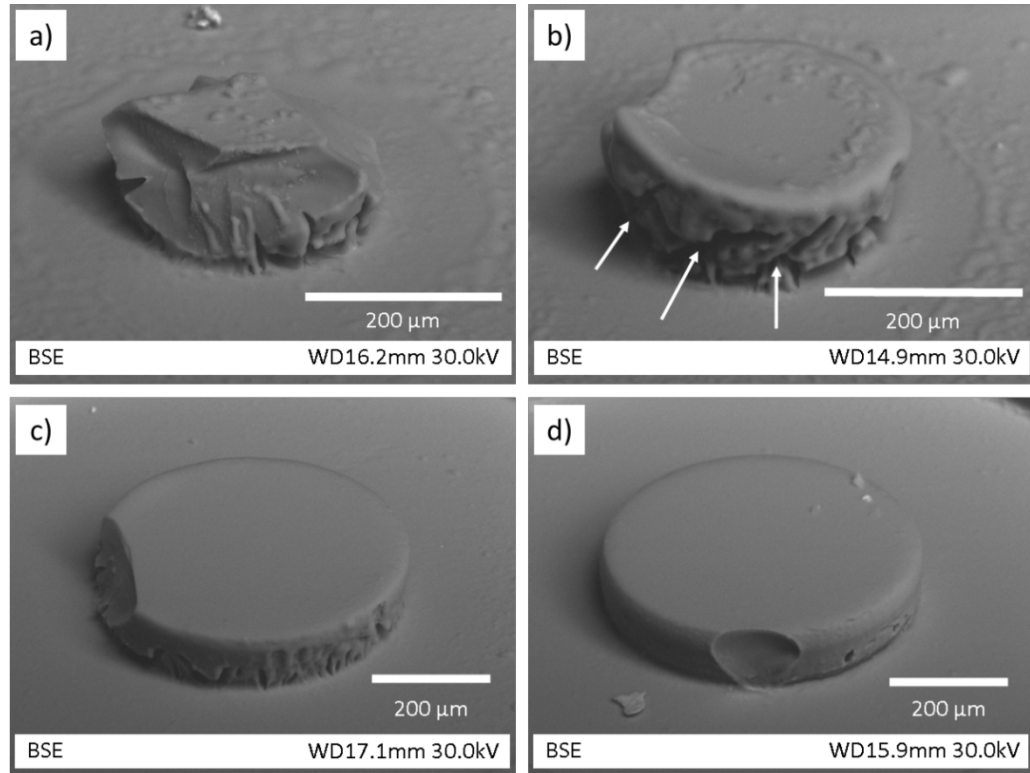


Figure 5-4: SEM images showing defects present on circular binding sites; a) and b) show Ø0.4 mm x 45° edge geometry, c) and d) show Ø0.6 mm x 45° edge geometry. White arrows indicate cracks in the structure caused by contraction due to evaporation in the curing process.

Typically for a self-assembly process the binding site shape will match that of the component face that it is aligning to. In order to achieve both axial and rotational alignment the simplest shape is that of a square. 0.5 x 0.5 mm and 1 x 1 mm square binding sites were manufactured and examined using the same fabrication and testing procedure as previously described. From the results presented in Figure 5-5 it can be seen that the resulting contact angles are similar to those seen for the circular binding sites, showing a shallower contact angle with increasing site size and steeper contact angle as the angle of the edge geometry decreases. The 1 x 1 mm binding site has a lower contact angle overall which is believed to be caused by the previously discussed effects of droplet diameter approaching the capillary length, and larger structures having a higher chance for the occurrence of edge defects from manufacturing due to their increased perimeter length.

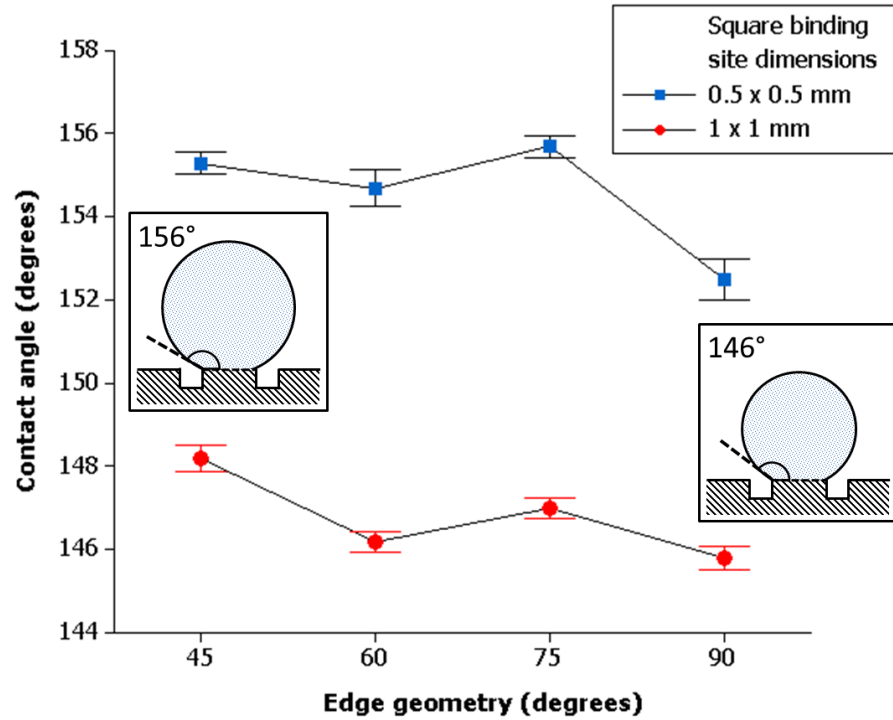


Figure 5-5: Contact angle of water droplets on square binding sites for different nominal edge geometries. Error bars display standard deviation.

Given the results observed for circular, 0.5 x 0.5, and 1 x 1 mm square binding sites, it was clear that the produced edge geometries may not match the nominal; designed geometries. In order to better understand how effective the production process was at achieving the nominal edge geometries square binding sites of 2 x 2 mm surrounded by 3 x 3 mm trenches were designed for the following experiments so they could be easily cross-sectioned and examined.

5.2 Cross-sectional analysis of structures

In order to assess the manufacturing processes ability to realise the desired edge geometries, square binding sites of 2 x 2 mm surrounded by 3 x 3 mm trenches were manufactured using the process outlined in section 3.2. Binding sites were cross-sectioned using a series of manual grinding operations on P400 to P4000 SiC paper, and examined by optical microscopy. The cross section perpendicularity was ensured by means of a parallel bar. Examples of

four binding sites can be seen in Figure 5-6 which shows images of actual edge geometry angles for the four nominal angles of 60° , 90° , 105° , and 135° .

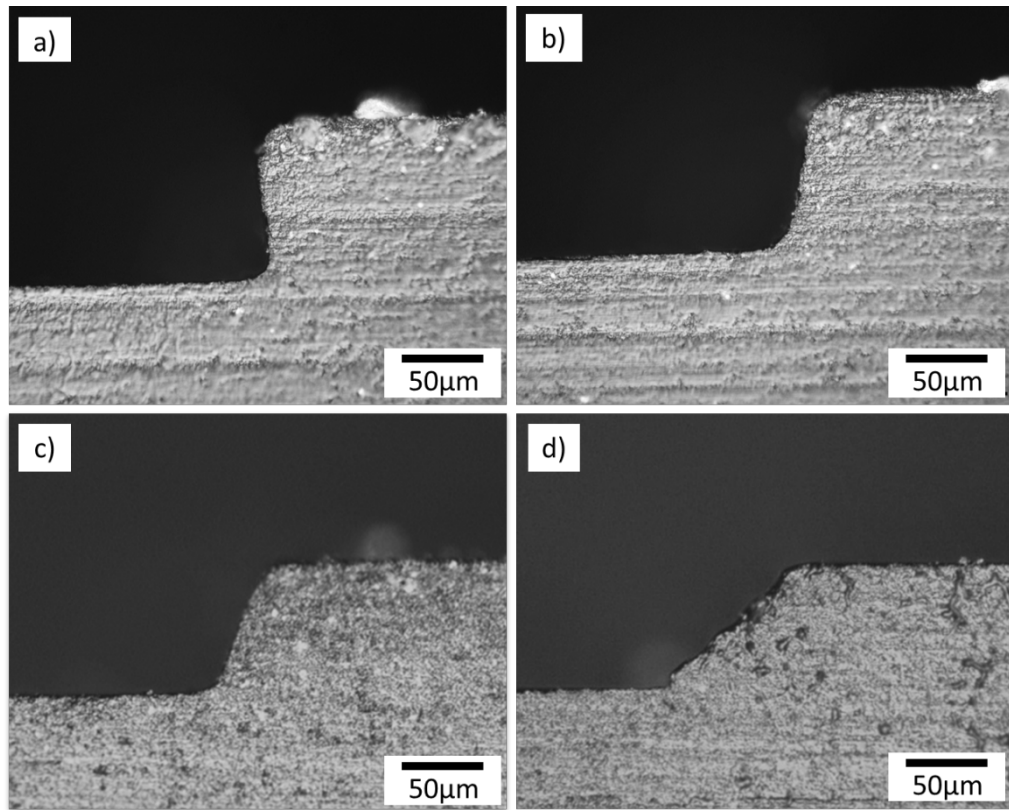


Figure 5-6: Optical microscope images of cross-sectioned binding sites. a) 60° nominal, b) 90° nominal, c) 105° nominal, and d) 135° nominal.

The average actual edge geometry is presented in Table 5-1 against the nominal angle, along with the standard deviation. From the data it can be seen that the manufacturing process struggles to recreate the nominal angles faithfully, with angles being greater than desired. This is more pronounced for angles $<90^\circ$ whereby the average measured angles were all close to $\sim 85^\circ$ regardless of the intended nominal angle. The large standard deviation observed for 45° nominal shows a high variability in the angles produced and correlates with the inconsistent results observed in section 5.1. This implies that it is more important to achieve a more consistent edge geometry, i.e. a low standard deviation, than it is to try and achieve very acute angle edge geometries.

<u>Nominal edge geometry (degrees)</u>	<u>Average actual edge geometry (degrees)</u>	<u>Standard deviation</u>
45	83	8.9
60	85	5.2
75	86	2.5
90	99	4.8
105	117	5.4
120	123	1.4
135	136	1.4

Table 5-1: Table summarising the average actual edge geometry compared to the nominal value.

5.3 Self-assembly of components using liquid surface tension

To study the capability of these sites to align parts by liquid surface tension a series of experiments were conducted where test components were placed onto the wetted sites with a large initial misalignment. The geometry of the sites was varied, and three distinct initial conditions were investigated, so that the ability to align both position and orientation could be considered. Square structures of 2 x 2 mm surrounded by 3 x 3 mm trenches 0.1 mm deep, were manufactured using the previously defined technique and nominal edge geometries from 45-135° were examined. The components used in the assembly tasks were rectangular prisms whose square bases matched those of the top surface of the binding sites, with dimensions 2 x 2 x 0.5 mm. Components were manufactured using the same material and fabrication techniques as detailed in section 3.2.1. Components were examined under an optical microscope and dimensions were within the expected 5% shrinkage inherent to the

manufacturing process. All component dimensions referred to in this chapter are nominal. A single liquid water droplet was applied to the surface of the topographical structure using the precision fluid dispenser described in section 3.2.4, and the component then placed by hand using tweezers. No special placement devices were used and as such the test represents a robust analysis of a challenging alignment task. To establish the variability of the human operator at depositing liquid to the binding sites, a random sample of 10 assembly cases were analysed whereby the average liquid volume was determined to be 204 nl with a standard deviation of 17 nl. Liquid volumes were measured using the technique described in section 3.2.7. The magnitudes of the combined misalignment in both x and y axis for droplet placement relative to the centre of the binding site was 216 μm with a standard deviation of 53 μm .

The three assembly cases examined in this work are illustrated in Figure 5-7: a) x-offset, where the component was offset from the target position by 500 μm along the x-axis (25% of the binding site dimension); b) twist-offset, where the component was positioned over the centre of the binding site, but rotated by 35° about the z-axis; and finally c) droplet-misalignment, where the liquid droplet was placed in the corner of the binding site and the component released directly over the droplet.

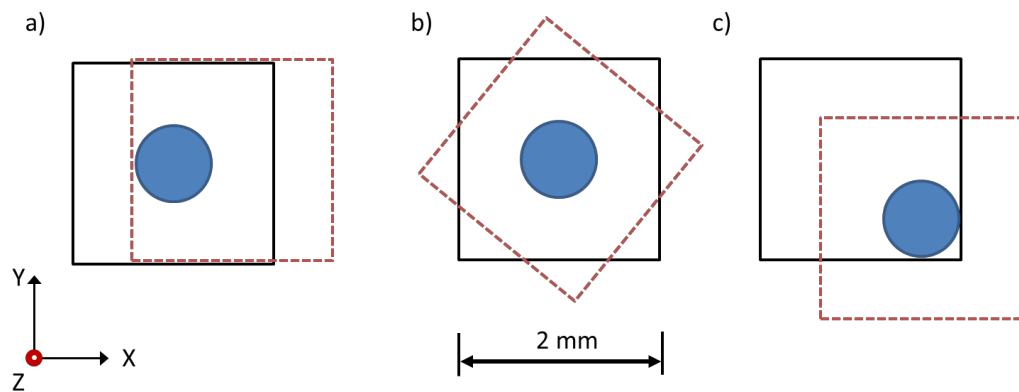


Figure 5-7: Schematic showing the three assembly cases examined in this work. Dotted line represents release position for component: a) x-offset, b) twist-offset, and c) droplet misalignment. Nominal component dimensions 2 x 2 x 0.5 mm.

For all cases we were interested in the linear alignment capabilities of the structures when components were subjected to large initial misalignments. All assembly cases were carried out across the full range of edge geometries and repeated ten times each (N=10). This information is summarised in Table 5-2.

<u>Case</u>	<u>Edge geometry (degrees)</u>	<u>Nominal component offset</u>	<u>Actual component offset</u>	<u>Standard deviation</u>
a)	45 (83), 60 (85), 75 (86), 90 (99), 105 (117), 120 (123), 135 (136)	500 μm	574 μm	29 μm
b)	45 (83), 60 (85), 75 (86), 90 (99), 105 (117), 120 (123), 135 (136)	35°	35.3°	1.3°
c)	45 (83), 60 (85), 75 (86), 90 (99), 105 (117), 120 (123), 135 (136)	-	691 μm	90 μm

Table 5-2: Summary of self-assembly tests carried out. Edge geometry represents nominal angle, with corresponding measured actual angle shown in brackets.

Once more, a random sample of 10 results was examined for each assembly case to assess the repeatability of component release position. For *case a)* the average x-offset was 574 μm with a standard deviation of 29 μm . For assembly *case b)* the average angle of release was 35.3°, standard deviation 1.3°. Repeatability of *case c)* was determined by calculating the magnitude of offset in both x and y axes between the component and binding site centres. This was found to be 691 μm with standard deviation of 90 μm .

The assembly process was recorded using the aforementioned acquisition techniques (section 3.2.7). Final assembly misalignment of the components was analysed using ImageJ software, with an x-y coordinate recorded for the difference between the component and binding site centres (section 3.2.7). To determine the precision of the measurement system, a known component was

measured 20 times and the repeatability of the system was determined to be ± 3 μm . An example of the assembly process can be seen in the image sequence below (Figure 5-8). The sequence is a series of optical microscope images for assembly *case b)*, where the component has an initial rotational misalignment from the binding site.

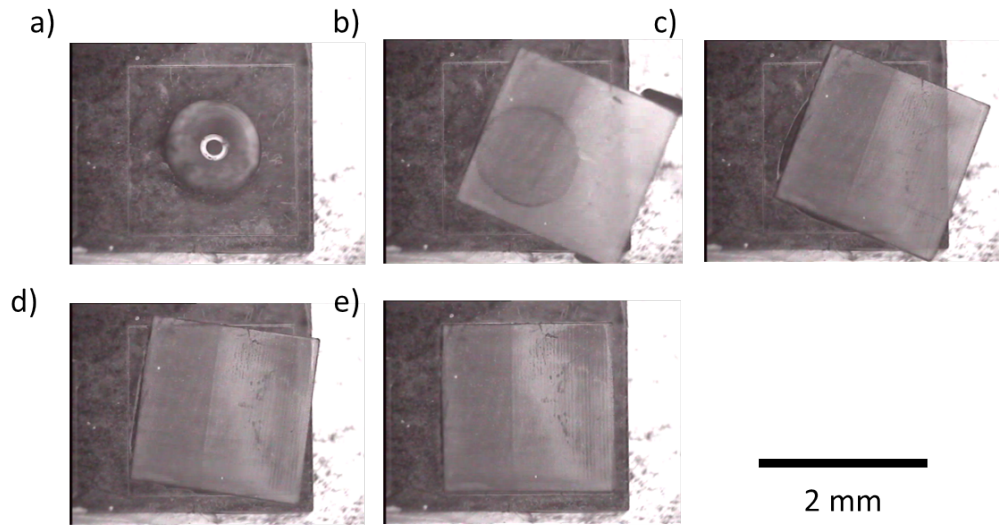


Figure 5-8: Optical microscope sequence for assembly *case b)*, twist misalignment of $2 \times 2 \times 0.5\text{mm}$ component. From left to right: a) liquid droplet on binding site, b) component placed with initial rotational misalignment, c) liquid droplet begins to wet to component, d) component moves into position, e) assembly process complete and component aligned with binding site.

Coordinate data for *case a)* x-offset, are displayed in the scatter plot, and the combined magnitudes of the misalignments in x and y axes in the boxplot in Figure 5-9 a) and b) respectively. From the data it can be seen that the magnitude of misalignment is significantly higher for edge geometries greater than 100° , with the data also being more spread. This indicates that the assembly process is considerably less reliable than for binding sites which have edge geometries of 100° or less. The full data for *case b)* and *case c)* are presented as scatter plots and boxplots in APPENDIX A.

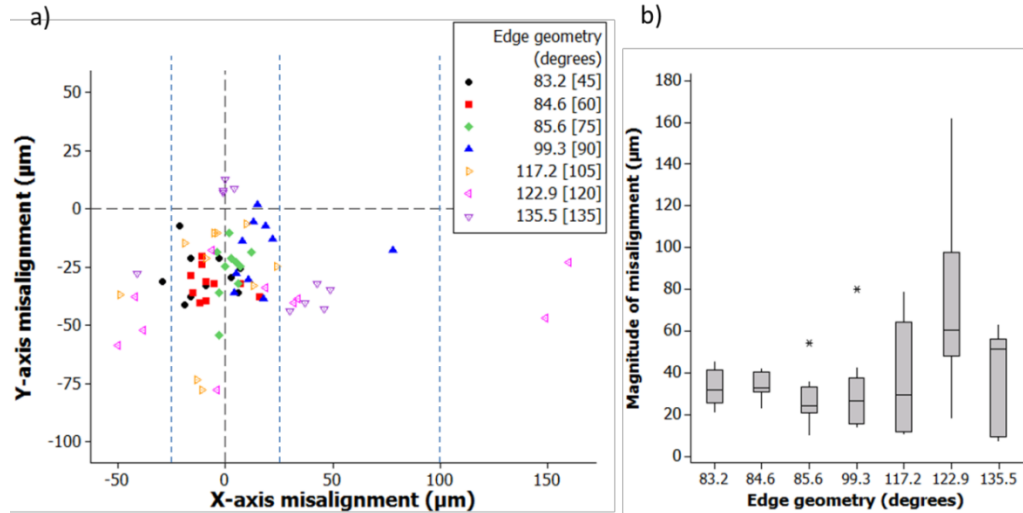


Figure 5-9: Assembly results for x-offset tests: a) scatter plot and b) box plot. Dotted lines indicate threshold regions of 25 and 100 μm misalignment in the x-axis. Numbers in brackets represent the nominal edge geometries. Asterisks indicate outliers in the data.

Figure 5-9 shows the component displacement considered as a magnitude against the edge geometry condition. It can be seen from the analytical solution for combined lateral misalignment presented in Chapter 6, section 6.3, that for misalignments less than 100 μm the surface energy is linearly proportional to displacement, and the contribution of the misalignments in the x axis and y axis can be summed in quadrature. As such displacements less than 100 μm can reasonably be represented by displacement magnitude, greatly simplifying the discussion of the effect of edge geometry.

Rather than consider the data presented in Figure 5-9 as a whole, it is convenient to consider the binding sites for their capability to achieve particular tolerances of assembled precision. Two threshold values have been selected, 25 μm and 100 μm of precision, and the effectiveness of the binding sites were evaluated against these thresholds, results shown in Figure 5-10. For *case a)* the threshold was applied to the x-axis only, and to both x and y-axes for *cases b)* and *case c)*. From Figure 5-10 it can be seen that the greatest capacity for alignment was realised for structures with an actual edge geometry $<100^\circ$. The structures with 45° nominal edge geometries are an exception however, with lower success rates observed at both thresholds across the three assembly cases. This is believed to be due to the high variability in the actual

manufactured angle which can be seen by the high standard deviation in Table 5-1. For structures with actual edge geometries greater than 100° the success rate is much lower and the assembly procedure becomes less reliable. Even though the success rate is still high in *case a*), looking at the box plot in Figure 5-9 b) it can be seen that the magnitudes of the misalignments are much higher as well as the standard deviation of data. Sites with actual edge geometries $>100^\circ$ do however show the capability to provide alignment when considered against the threshold criteria, see Figure 5-10.

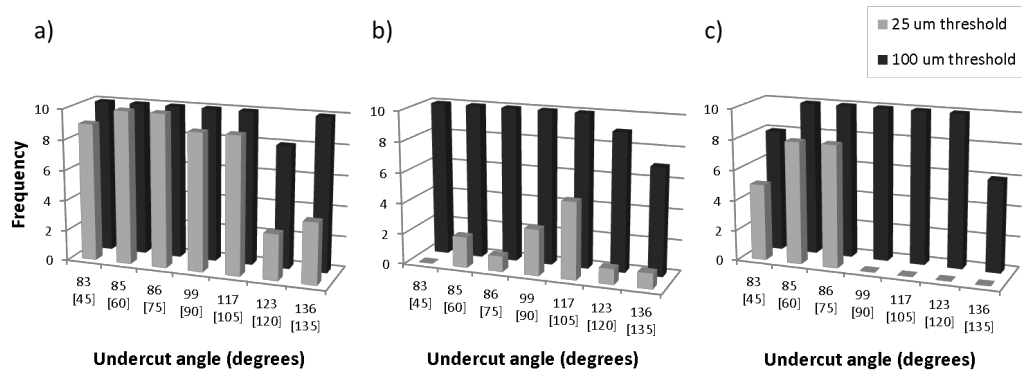


Figure 5-10: Bar charts showing component assembly success rates for misalignments less than or equal to the given threshold in both x and y axis: a) x-offset, b) twist-offset, c) droplet misalignment. X-axis displays the measured edge geometry, with corresponding nominal angle shown in brackets.

For sites with edge geometries $>100^\circ$ there is significant standard deviation in the final misalignment. This makes the interpretation of this data very difficult, which is an aspect not captured by the threshold plots. It was decided to exclude this data from further analysis and focus on structures with actual edge geometries below 100° , i.e. nominal angles of 45° , 60° , 75° and 90° , where similar trends might be observed but with less significant standard deviation.

Although this study was primarily interested in linear alignment capabilities, it was observed that all components aligned within $\sim 2^\circ$ about the z-axis, even when under extreme rotational misalignment in *case b*). The only exception to this was the components that failed to align altogether, and these were the cases that fell outside the 100 μm threshold. The findings presented in this section

are in agreement with the results in section 5.1 which showed a significant reduction in contact angle achieved when the edge geometry was increased beyond 90° . Comparison of the initial contact angle measurements and the alignment experiments would suggest that the liquid contact angle observed for isolated droplets is a useful indicator of performance in alignment tasks.

Excluding the data outside the $100\ \mu\text{m}$ misalignment threshold, an analysis of the spread of successful assembly cases can be observed. From the data (Figure 5-10 and Figure 5-11) it can be seen that structures with an edge geometry less than 90° (excluding 45° nominal) have the most consistent set of results having a combined success rate of 96.7%, and a fairly even spread of data across the three different assembly cases. For structures having a 45° and 90° nominal edge geometry the misalignment magnitudes are similar to those for $<90^\circ$. However the failure rate is higher meaning the data set is therefore smaller and less reliable. The mean misalignment for angles $>90^\circ$ in *case c*) is much greater, as is the range of results. Based on the box plot in Figure 5-10 c), it can be seen that there were no successful assembly cases at the $25\ \mu\text{m}$ threshold for structures with edge geometries $>90^\circ$. This indicates the poor alignment capability of the $>90^\circ$ edge geometries when the assembly task becomes more challenging.

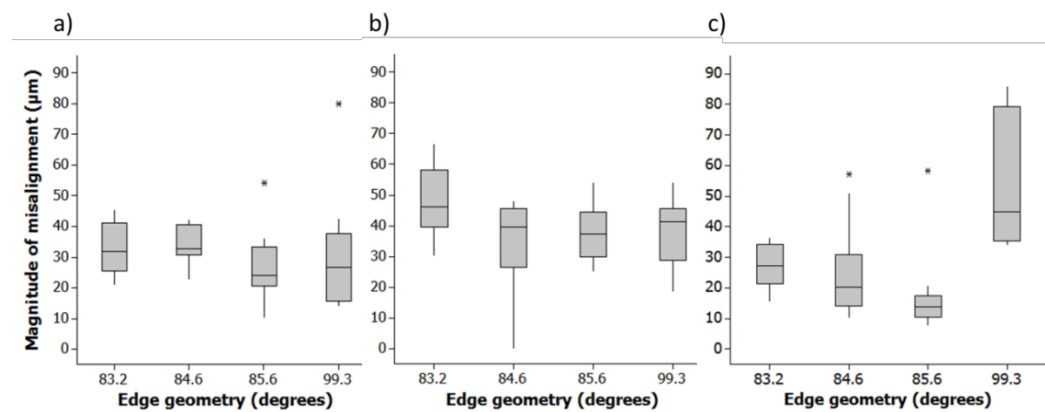


Figure 5-11: Boxplots of assembly results showing magnitude of component misalignment in both x and y axis against binding site edge geometry for assembly cases falling within the $\pm 100\ \mu\text{m}$ threshold: a) x-offset, b) twist-offset, c) droplet misalignment. Asterisks indicate outliers in the data.

In order to better understand this variation in performance scanning electron microscopy (SEM) was performed to investigate the binding sites. This revealed that defects had been introduced in the fabrication of the structures with 45° nominal edge geometries. Figure 5-12 a) shows the correctly fabricated structure, however the opposite edge of the same binding site, displayed in Figure 5-12 b) shows that the structure had not formed correctly and material had gathered to form a radius.

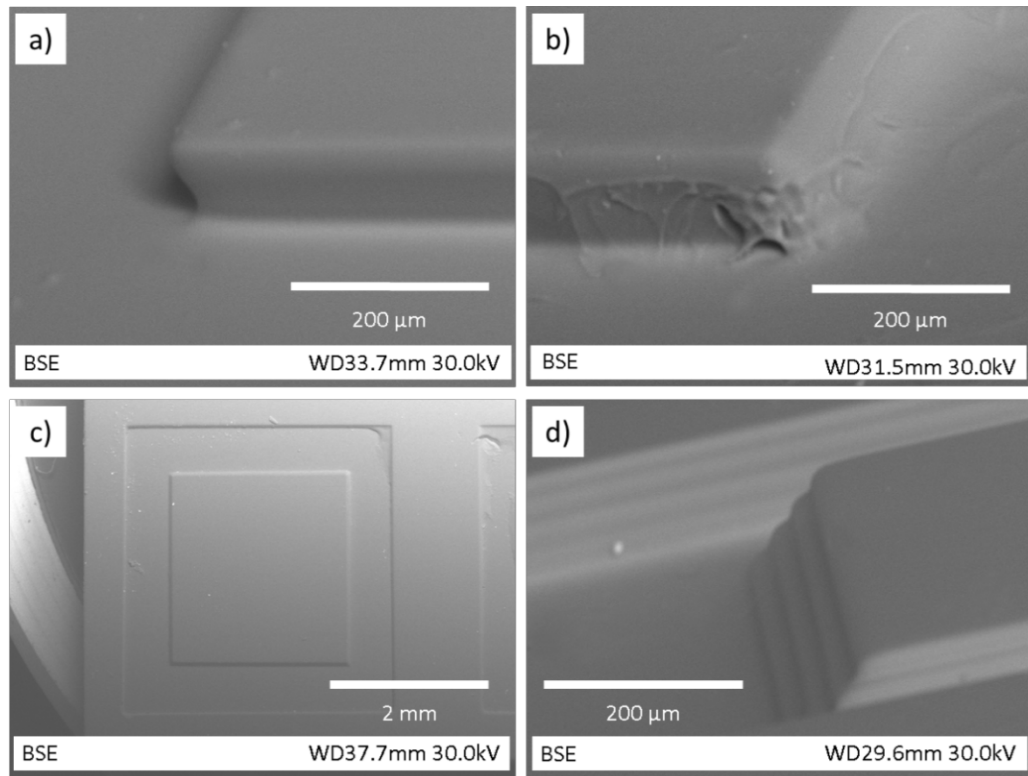


Figure 5-12: SEM images of 2 x 2 mm assembly structures. a) 45° nominal edge geometry, b) 45° nominal with incorrectly manufactured edge geometry, c) top-down view of 105° structure, d) 135° structure clearly showing stepping of individual $25\ \mu\text{m}$ layers.

These defects could explain the failed assembly attempts observed for the 45° nominal edge geometries and is in agreement with the high standard deviation observed with the cross-sectional analysis in section 0. Figure 5-12 d) illustrates the defects in the sites produced with edge geometries $>90^\circ$. The individual $25\ \mu\text{m}$ layers can clearly be seen to have produced step features, and that a smooth incline was not achieved. From the images obtained it would appear that each layer was effectively only a straight 90° edge offering no

benefit going beyond a complete 90° edge geometry. Experimental observations found that during assembly the liquid would meet the edge of the binding site and overflow, proceeding to the next edge on the 25 µm layer below, and so on. It was seen that when the liquid had overflowed, the component would align to the geometry of the lower layers. This would explain the consistently high misalignments observed, and the large number of cases falling outside of the assembly thresholds.

5.4 Experimental observations of liquid droplet response

A series of novel experiments were conducted using an Agilent G200 nanoindenter machine at the University of Leicester. A custom designed indenter tip was additively manufactured using the EnvisionTec Perfactory (described in chapter 3, section 3.2.1) and used to replace the existing tip with a profile matching the binding site geometries typical of those investigated throughout this thesis. Full details of the experimental procedure can be found in chapter 3, section 3.2.10.

A series of five background readings were carried out without placing any liquid on the binding site in order to establish the behaviour of the force sensors of the nanoindenter. These were divided into two sections for the approach and return motion of the indenter tip. A 5th order polynomial was fitted to each data set and used to extract the background readings from the test data. These can be found in APPENDIX A.

A plot of the load against the distance of the indenter tip from the binding site surface for a liquid volume of 360 nl is presented in Figure 5-13. Four reference lines have been added to identify the important stages of the test procedure which are believed to occur. At stage 1 the indenter tip makes contact with the liquid droplet on the binding site top surface. At this point the liquid begins to form a bridge between the two faces, generating a tensile force. This acts to pull the indenter tip towards the binding site resulting in a negative load. At stage 2 the liquid is now fully wetted to both the indenter tip and the binding site top surface. The point of inflection is the equilibrium position for

the indenter tip. The liquid then enters a compressive state as the indenter tip continues to travel towards the binding site surface before reaching the maximum load at stage 3. Past this point the liquid overflows the binding site which can be seen as a drop in the load as the indenter tip continues to move. The slope then starts to rise again before stage 4 as the indenter tip now compresses the small amount of remaining liquid on the binding site surface. At stage 4 the tip makes contact with the surface and there is a sharp rise in the load as mechanical contact between the two surfaces is made. It is important to note that it was not possible to view the experimental procedure under a microscope during the measurements. The points of interest discussed and highlighted in Figure 5-13 are inferred from the collected data based on the authors observations made during the experimental work, and from previous behaviour observed from the self-assembly experiments conducted in section 5.3.

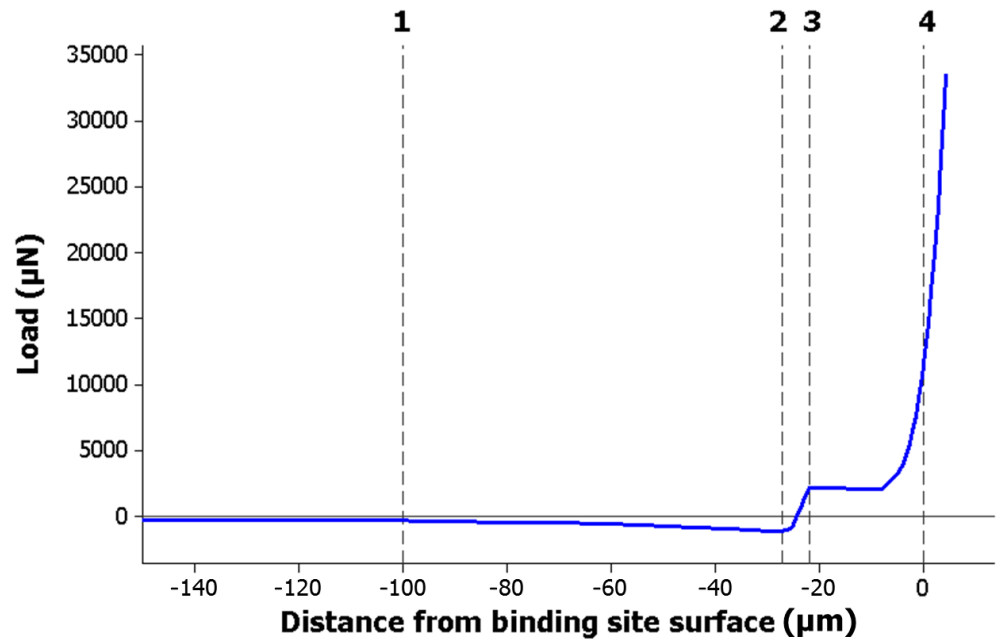


Figure 5-13: Plot of load against distance from binding site surface for test conducted using Agilent G200 nanoindenter. Binding site dimensions 1.75 x 1.75 x 0.1 mm with 80° edge geometry and liquid volume 360 nL. Dotted lines are for reference which show: 1) Indenter tip makes contact with liquid droplet, 2) Liquid droplet fully wetted to binding site and indenter tip, enters compressive state, 3) Droplet overflows binding site, 4) Contact of indenter tip with binding site surface.

Plotting the data for four tests of similar liquid volume allows a comparison between the loading characteristics (Figure 5-14). Dotted lines have been added to the figure to highlight the gradient of the slope when the liquid droplet is in compression before overflowing the binding site top surface.

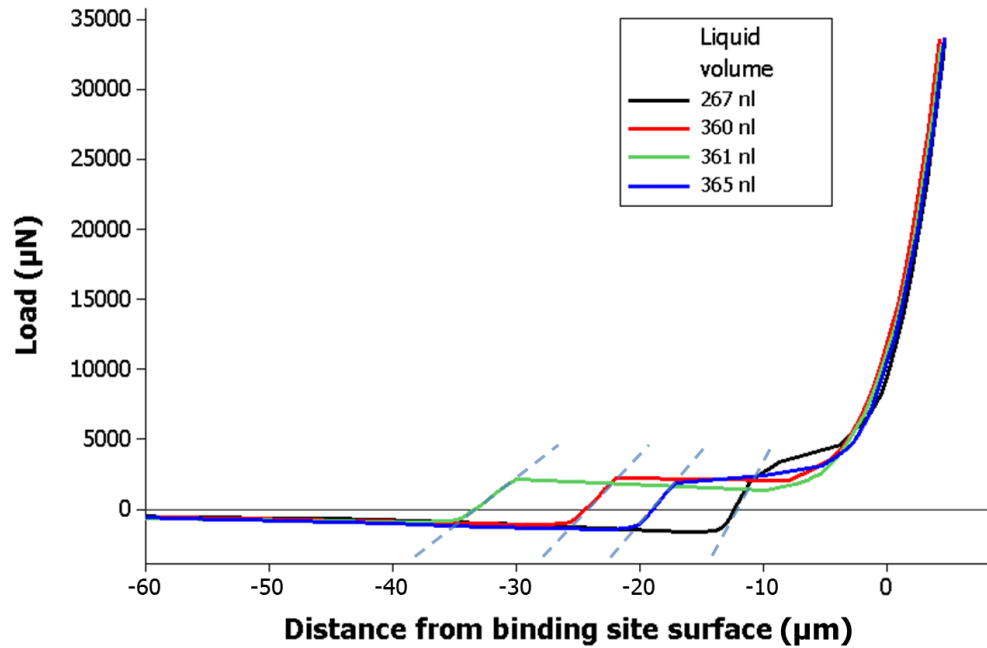


Figure 5-14: Plot of load against distance from binding site surface for test conducted using Agilent G200 nanoindenter. Binding site dimensions 1.75 x 1.75 x 0.1 mm with 80° edge geometry for a range of liquid volumes. Dotted lines used to highlight the gradient of the compressive portion of the loading before liquid overflow.

The data show that for the three liquid volumes 360, 361 and 365 nl similar loading profiles occurred. After the maximum compressive load was reached of approximately 3 – 5 mN there was a plateau as the liquid overflowed the binding site before the load rose again due to compression of the remaining liquid and finally contacting the surface. For the liquid volume of 267 nl the plateau region occurred over a much shorter distance which is consistent with the reduced liquid volume. The distance from the binding site surface at which the liquid droplet passed through the equilibrium position and into the compressive state, as well as the length of the plateau region are directly related to the volume of liquid applied to the binding site surface. The aforementioned dotted lines which have been overlaid on the plot show the

linear portion of the spring constant for the liquid droplet. It can be seen that the maximum compressive load achieved is similar for all liquid volumes, however the distance over which this occurred was shorter for the lower liquid volume indicating a stiffer response.

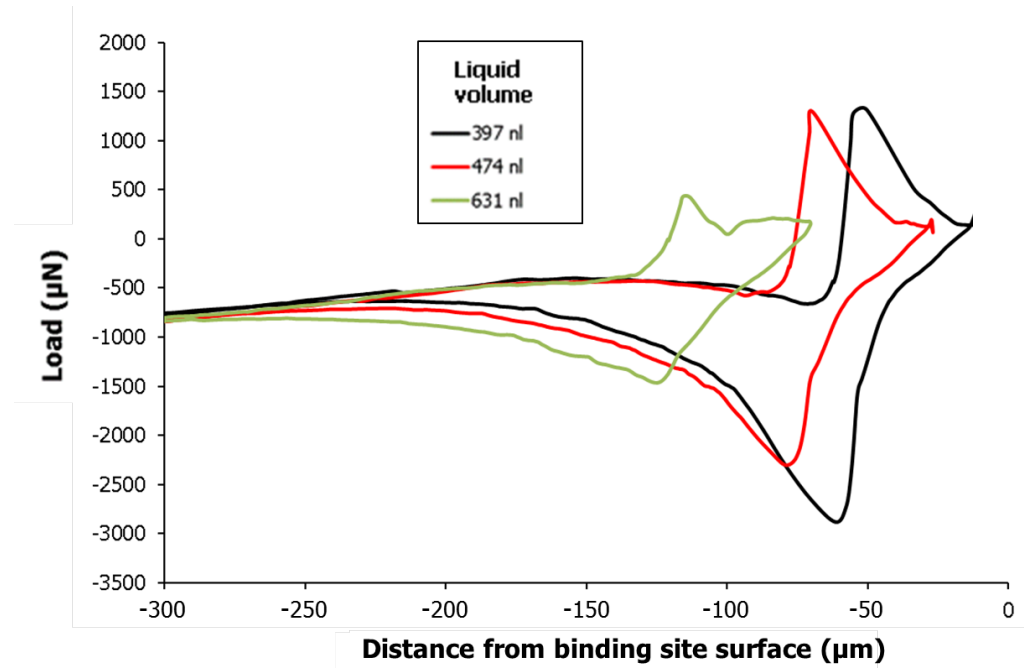


Figure 5-15: Plot of load against distance from binding site surface for test conducted using Agilent G200 nanoindenter. Binding site dimensions 1.75 x 1.75 x 0.1 mm with 80° edge geometry for a range of liquid volumes.

The measurement strategy was altered to reduce distance travelled by the indenter tip after detecting the liquid droplet and not fully contact the binding site surface. The measurement strategy was also altered to record the load during the unloading (reverse) stage. The load profiles for three liquid volumes are presented in Figure 5-15. For each liquid volume a similar initial profile is seen to that of the data presented in Figure 5-14 whereby a point of inflection is reached before compressing the liquid droplet observed by a rise in the load. The unloading profile of the data is believed to be caused by contact angle hysteresis of the liquid droplet (see chapter 2, section 2.4.10). This is caused by the pinning of the liquid triple contact line (TCL) on local surface defects, resulting in a lower receding contact angle and an increase in the tensile force exerted by the droplet.

5.5 Summary

This chapter investigated the use of additively manufactured micro structures for the self-assembly of components using liquid surface tension of water droplets. Test components were manufactured on an EnvisionTec Perfactory Mini-Multi lens projection stereolithography machine. This work has demonstrated that component alignment relies on careful constraint of droplet position and shape. Droplet shape on circular and square binding sites with varying degrees of edge geometry was investigated and significant increases in contact angle of liquid water droplets were observed, with contact angles up to 158° achieved compared to 70° when placed on the plain substrate. This suggests that edge geometry has a dramatic effect on the ability to pin the TCL. A decrease in the contact angle was observed for structures where the nominal edge geometry was greater than 90° , compared to angles achieved for structures with nominal edge geometries less than 90° , implying that $>90^\circ$ offer significantly less constraint. It was observed that if the major droplet dimension approached that of the capillary length then lower maximum contact angles were achieved, attributable to gravitational force playing a proportionally greater role.

Cross-sectional analysis of the structures revealed that the manufacturing process struggled to faithfully recreate the nominal angles, with actual edge geometries tending to be oversized. SEM imaging showed a distinct stepping of the individual layers for structures with actual edge geometries $>100^\circ$ which tended to ruin the self-alignment process if the droplet overflowed the top layer of the binding site.

Despite the discrepancy between nominal and actual edge geometries all structures displayed a capacity for alignment at the $100\text{ }\mu\text{m}$ threshold for the three assembly cases. Clear benefits were observed for structures with actual edge geometries $<90^\circ$ (excluding 45° nominal) which achieved repeatable alignment at the $25\text{ }\mu\text{m}$ threshold, with a mean misalignment of $31\text{ }\mu\text{m}$ and $14\text{ }\mu\text{m}$ standard deviation. The results also suggested that it was more important

to achieve a lower standard deviation in the edge geometry than it was to achieve highly undercut angles.

An investigation of liquid droplet response was conducted via a novel set of experiments using an Agilent G200 nanoindenter machine. Data showed that specific events could be identified during the loading and unloading of a liquid droplet placed on a binding site when using an additively manufactured indenter tip. Maximum compressive loads for the liquid droplet before overflow of the binding site were $\sim 3 - 5$ mN. Variations in the data between the loading and unloading profiles was attributed to contact angle hysteresis caused by pinning of the TCL on local surface defects creating a lower receding contact angle and therefore a higher tensile force.

The work presented in this chapter has shown that even without a well-defined sharp edge, additional materials, or coatings to surfaces, accurate and repeatable assembly of micro components using liquid surface tension is achievable. It has clearly demonstrated that additively manufactured micro devices can be easily modified to include liquid binding sites, and that this makes the use of liquid surface tension for assembly of such devices an attractive process.

In the following chapter the use of a free-to-use software tool for the numerical modelling of surfaces shaped by surface tension is introduced.

Chapter 6

6 NUMERICAL MODELLING OF SPRING CONSTANTS USING SURFACE EVOLVER

Industrially manufactured products are typically assemblies made up of many separate and often dissimilar components. The assembly techniques required to realise these finished items are therefore of key importance to product generation. Liquid self-assembly of components is an attractive alternative to traditional robotic pick-and-place techniques as it can offer very high final positional accuracy with fairly coarse initial placement. This means lower cost, faster pick-and-place systems, or the replacement of robotic pick and place with manual pick-and-place; leading to the advantages of either increased system flexibility, or reduced cost and higher throughput.

Liquid self-assembly utilises the placement of a component onto a liquid droplet on a well-defined structure known as a binding site. When the component is misaligned with the binding site the surface area of the liquid droplet becomes deformed. This deformation results in an increase in the surface area of the liquid droplet, and therefore an increase in surface energy. This excess surface energy can be minimised by the movement of the component to a position where it is well aligned with the binding site.

Understanding the behaviour of components in the self-assembly process is of key importance to designing successful assemblies. There are a number of analytical methods presented in the literature by which to describe simple liquid droplet arrangements [85, 181, 182]. However these are difficult to apply when geometries become more complex. One method that has been employed by a number of researchers is the free-to-use software Surface Evolver. Developed by K. Brakke, Surface Evolver (SE) allows the modelling of shapes formed by surface tension and other energies. The Surface Evolver has a steep learning curve with models created via text-based data files. The steps necessary in creating these data files, as well as the processing of results are particularly time consuming. This means that the barrier to entry is

particularly high, and its acceptance as part of the design process in an industrial environment is unlikely.

This chapter presents the work undertaken to establish a set of spring constants for a liquid droplet when in contact with a component. The work is conducted using the free-to-use software Surface Evolver. The simulations presented consider the component while under different states of misalignment from the equilibrium position, and provide non-linear spring constants for these individual degrees of freedom of the component.

6.1 The physics and operation of Surface Evolver

Surface Evolver is a program which performs numerical modelling of surfaces shaped by surface tension and other energies, subject to applied constraints. Surfaces are represented as a series of triangles, defined by the user in a datafile. Surface Evolver performs iterative numerical estimation to ‘evolve’ the shape of surfaces to find the minimum energy state. The sources of energy considered by Surface Evolver during the evolution can be a combination of surface tension, gravitational energy, or user-defined surface integrals. An iteration is one evolution step, which is determined through a three-step process: Firstly, the force on each vertex is calculated using the gradient of the total energy of the surface using the gradient descent method, based on the position of the vertex and the user defined energy sources. Secondly, the force is subjected to any applied constraints. Thirdly, the motion of the vertex is determined by multiplying the calculated force by a global scale factor. This is performed for each vertex of the surface, the vertex is then moved to this new coordinate based on the step size, scale factor and any constraints it is subjected to.

For readers who are unfamiliar with the Surface Evolver software, an introduction to the programs functions, as well as recommendations based on the authors’ own experience, can be found in APPENDIX C.

6.2 Modelling approach

In this chapter a series of models were produced and simulations conducted that evaluate a simple component on a binding site, and investigate the forces produced by misalignment. These simulations were designed in order to isolate the forces acting on the system for each of the 6 degrees of freedom (DOF) of the component part. The cases considered are lateral displacement (which covers misalignment in x and y axes), vertical displacement (misalignment in z axis), torsional displacement (misalignment around z axis), and finally tipping displacement (misalignment around x and y axes). In order to simplify the models the following assumptions were made: Firstly it is assumed that the liquid volume remains constant throughout the assembly processes and that no evaporation occurs. Secondly it is assumed that the assembly liquid has fully wetted both the binding site and component assembly faces and is pinned along their perimeters. Thirdly, that the component is placed carefully and may be considered to begin the simulation with zero velocity.

A series of Surface Evolver simulations and simple analytical approximations have been presented previously in the literature by Berthier et. al [85] to investigate the assembly of 5 x 5 x 0.75 mm microchips onto chemically altered hydrophilic binding sites of dimensions 5 x 5 mm located on silicon wafers. The model used in this section was developed by K.Brakke and adapted to a geometry that is relevant to the structures investigated in this thesis. The model data file can be found in APPENDIX E. Establishing the forces for each isolated DOF is of particular interest to micro assembly tasks where the component may be misaligned in one particular axis. For example the experimental work conducted in chapter 5, section 5.3 investigated discrete misalignment cases for a component assembled onto a binding site using a liquid droplet of water. For one assembly case the component misalignment was purely lateral, and for another case, was purely torsional. Conducting a numerical investigation using Surface Evolver allows comparisons to be drawn to the experimental findings previously presented in this thesis. Establishing the forces for each DOF using Surface Evolver allows them to be applied to the

assembly of more complex geometries in a computer aided engineering (CAE) package, which would otherwise be extremely difficult and time consuming to simulate effectively in Surface Evolver. The integration of the forces into a commercially available CAE package is presented later in chapter 8, section 8.2.3.

All models presented in this chapter are in line with previous geometries explored in chapter 5, section 5.3: The square binding site has a top surface of 2 x 2 mm, and the components are rectangular prisms having a face in contact with the liquid droplet of 2 x 2 mm. The liquid used in the models was water with surface tension of 72.8×10^{-3} N/m. The contact angle of the liquid with the solid surface was 70 degrees which was experimentally determined in chapter 3, section 3.2.6. Three different liquid volumes were simulated: 250, 500 and 1000 nl. The distance between the component and binding site was set as the liquid volume divided by the area of the binding site top surface. This information is summarised in Table 6-1.

Binding site dimensions:	2 x 2 mm square binding site
Component dimensions:	2 x 2 x 0.5 mm
Assembly liquid:	Water, surface tension 72.8 mN/m
Contact angle:	70 degrees
Liquid volumes:	250 nl, 500 nl, 1000 nl

Table 6-1: Summary of model parameters.

For each simulation the geometry was held in a fixed position and the resulting resolved final surface energy recorded. As an example, in the case of lateral misalignment of the component, the x-coordinate of the component vertices was defined using a variable, which was then incremented for each new

simulation. Using this method a final surface energy for each lateral position of the component was then obtained. As each simulation requires its own data file it is easy to see how the batch generation and processing of these files is a necessity.

Plotting the surface energy against the degree of misalignment for each case reveals how the energy in the system changes in relation to the misalignment. Taking the differential of the surface energy with respect to the misalignment gives the restoring force exerted by the liquid droplet acting on the component.

A rendered image of the Surface Evolver model illustrating the four displacement cases is presented below in Figure 6-1. These four cases make up the 6-DOF for the model; vertical displacement along the z-axis, rotational displacement around the z-axis (twisting), lateral displacement along the x and y axis, and rotational displacement acting around the x and y axis (tipping). The yellow represents the surface of the component which is in contact with the assembly liquid (blue).

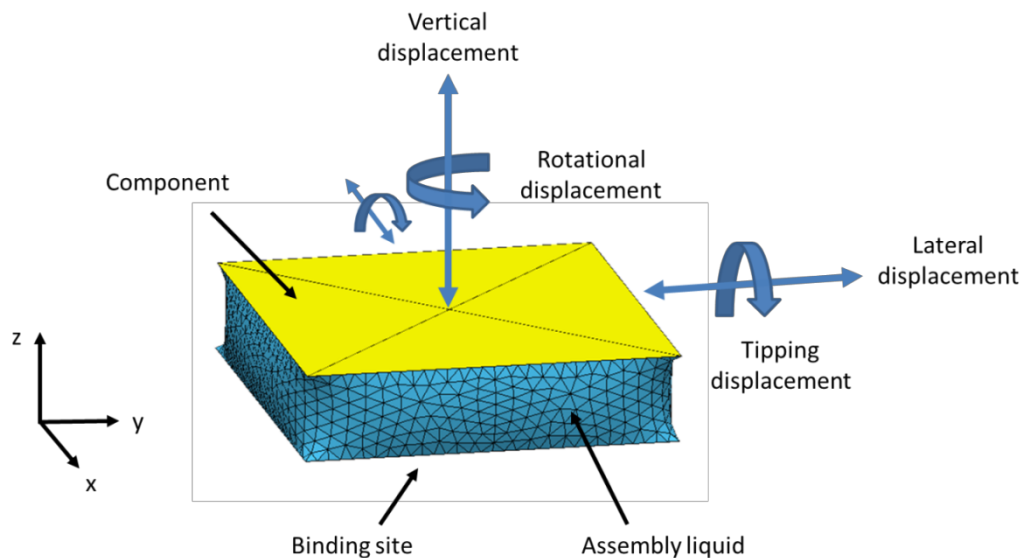


Figure 6-1: Diagram illustrating the modelling approach, with the four different displacement cases labelled accordingly.

A data file has been constructed to represent the desired geometry and permit easy control of component misalignment. Individual macros were written to allow each discrete displacement case to be investigated separately.

The model has been constructed using the CGS (centimetre, gram, second) system of units. This is to keep the numbers within the data file close to 1, as this is the preferred format for Surface Evolver. Once the motion of a vertex is calculated for each iteration the direction must be multiplied by a scale factor to compute the actual motion. The scale limit of the system sets an upper bound on the scale factor and is set to $1/\text{surface tension value}$. This is recommended in the Surface Evolver documentation if the surface tension of the assembly liquid is the dominant force of the system.

In the following subsections the four individual cases will be introduced along with an explanation of any specific assumptions or constraints applied to the particular model.

6.3 Lateral displacement

This Surface Evolver simulation measures the stiffness characteristic of a liquid droplet undergoing lateral displacement as a component is given a misalignment in either the x or y-axis.

The force needed to extend or compress a spring by a distance, is proportional to that distance, and is given by Hooke's Law:

$$F = -kx \quad (6-1)$$

Where F is the force, x is the displacement, and k is the spring stiffness.

The potential energy stored in displacing a spring from its un-stretched length can be found by:

$$PE = \frac{1}{2}kx^2 \quad (6-2)$$

The behaviour of the liquid droplet during component misalignment is analogous to that of a spring. The force exerted by the droplet on a component at a particular displacement can be found by differentiating the surface energy with respect to the displacement.

$$F_x = \frac{\partial(\gamma S)}{\partial x} \quad (6-3)$$

Where F is the force, γ is surface tension, S is the interfacial area, and x is the displacement.

Differentiating again with respect to the displacement allows the stiffness to be obtained:

$$k = \frac{\partial^2(\gamma S)}{\partial x^2} \quad (6-4)$$

In this series of simulations three liquid volumes were examined: 250, 500 and 1000 nL. The displacement of the component was simulated from zero misalignment i.e. perfectly aligned with the binding site, to 0.5 mm displacement in the x-axis in 5 μ m increments (Figure 6-2). This allowed the resolved lowest surface energy condition for each misalignment position to be determined.

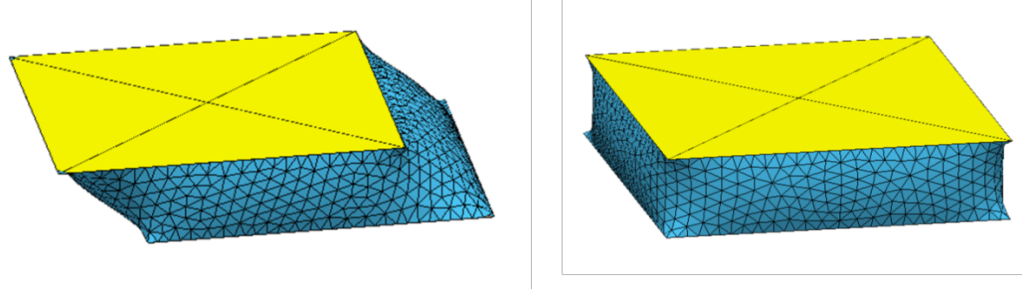


Figure 6-2: Rendered image of Surface Evolver model for the case of lateral misalignment. (Left) Component with an initial misalignment of 0.5 mm. (Right) Fully assembled component in equilibrium position.

Data files were generated by writing a batch script in Matlab which altered the component position in the x-axis by modifying the *xoffset* variable for each data file. Data files were then batch run in SE-FIT and their results extracted from the output file using a second Matlab script which identified the relevant lines.

The results were compared to a simple analytical solution which assumed the deformation of a planar interface (Figure 6-3). The surface energy of the liquid-air interface can be shown to be [85]:

$$E \approx 2\gamma Lh \left(1 + \sqrt{1 + \left(\frac{x}{h}\right)^2} \right) \quad (6-5)$$

Where γ is surface tension, L is the length of one side of the binding site, h is the distance between the binding site surface and component, and x is the component displacement (as illustrated in Figure 6-3).

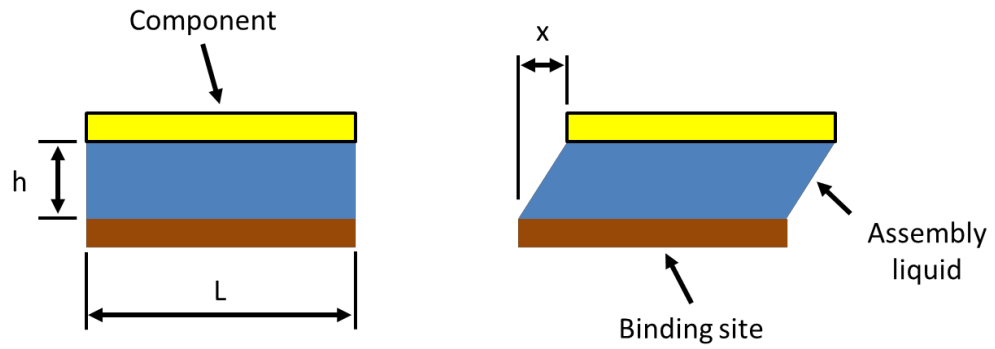


Figure 6-3: Diagram illustrating the definition of the analytical solution for lateral misalignment of a component.

The surface energy was plotted against misalignment position of the component for the three different liquid volumes (Figure 6-4). Solid lines represent the numerical solution calculated in Surface Evolver, and dotted lines represent the analytical solution obtained from equation (6-5). It can be seen that there is a slight difference between the two solutions caused by the approximation of the interface in the analytical solution which assumes that the surfaces remain planar (Figure 6-3). In contrast the numerical solution shows the interface to be shaped by the liquid-air surface tension, resulting in a minimal surface area (Figure 6-5).

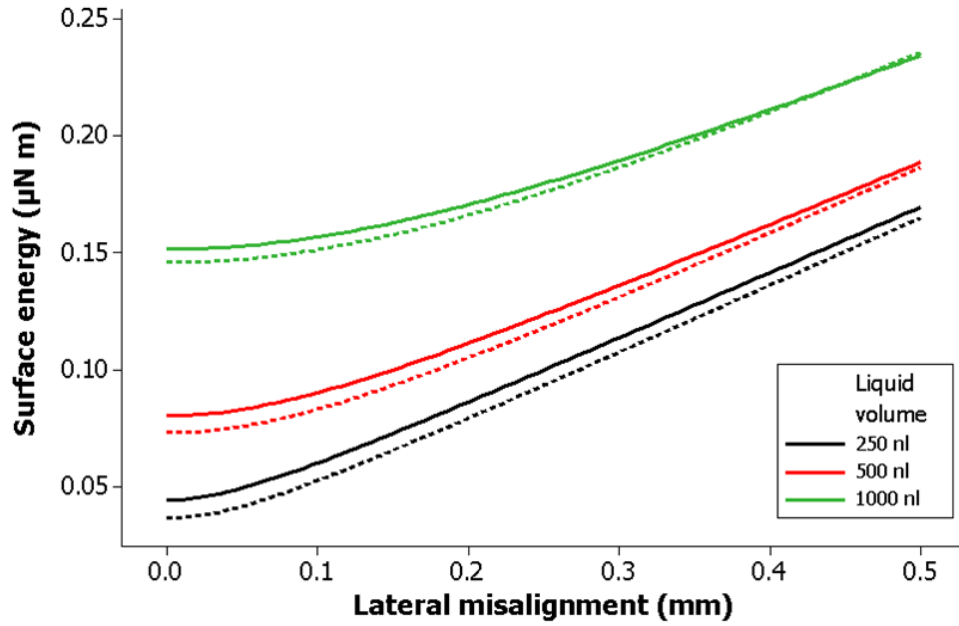


Figure 6-4: Plot of surface energy against component lateral misalignment for varying liquid volume. Solid lines show Surface Evolver numerical solution, dotted lines show analytical solution.

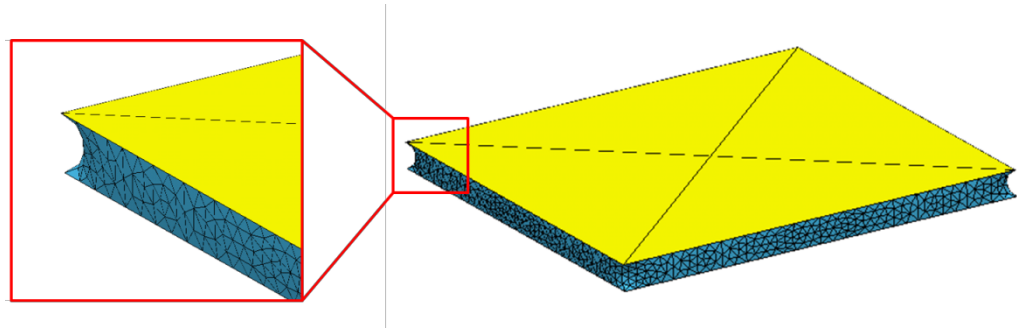


Figure 6-5: Rendered Surface Evolver image showing the liquid interface adopting a minimal surface area due to surface tension.

Data were imported into Matlab where a numerical differentiation was performed using a spline fit to obtain the restoring force exerted by the liquid droplet on the component. Data were then smoothed by fitting a 6th order polynomial. The Matlab script can be found in APPENDIX F. Results were compared to a simple analytical solution (equation (6-6)) [85] with restoring force plotted against lateral misalignment of component (Figure 6-6). Solid lines represent numerical Surface Evolver solution, and dotted lines show analytical solution.

$$F_x \approx -2\gamma L \frac{1}{\sqrt{1 + \left(\frac{h}{x}\right)^2}} \quad (6-6)$$

Where γ is surface tension, L is the length of one side of the binding site, h is the distance between the binding site surface and component, and x is the component displacement in the x -axis.

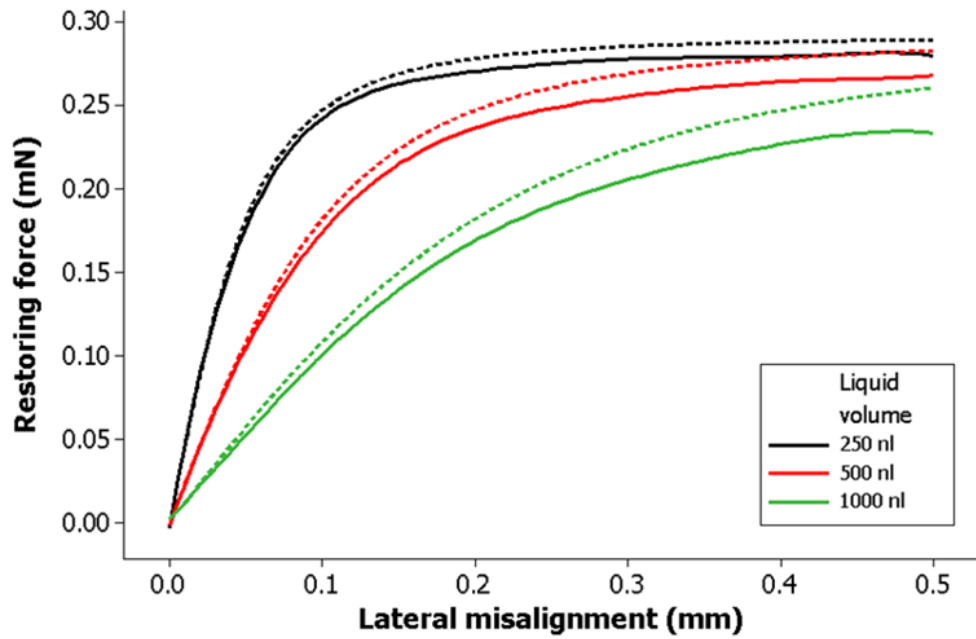


Figure 6-6: Plot of restoring force against component lateral misalignment for varying liquid volume. Solid lines show Surface Evolver numerical solution, dotted lines show analytical solution.

It can be seen that the numerical simulation results match the analytical solution well for both the surface energy and restoring force when plotted against the lateral component misalignment. Both numerical and analytical solutions show that a higher surface energy is seen for larger liquid volumes due to the increased interfacial area. Conversely higher restoring forces are observed for lower liquid volumes due to the relative rate of change in the shape of the interface as component misalignment increases. The restoring force can be seen to be fairly constant once the maximum force is reached regardless of increased component misalignment, showing that the liquid

droplet offers strong alignment capabilities over a large misalignment range for this DOF.

If the case is modified to consider simultaneous lateral misalignment in both the x and y axes, the analytical solution can be shown to be (APPENDIX G):

$$E = 2\gamma L \left(\sqrt{y^2 + h^2} + \sqrt{x^2 + h^2} \right) \quad (6-7)$$

Where γ is surface tension, L is the length of one side of the binding site, h is the distance between the binding site surface and component, and x and y are the component displacements in the x and y axes respectively.

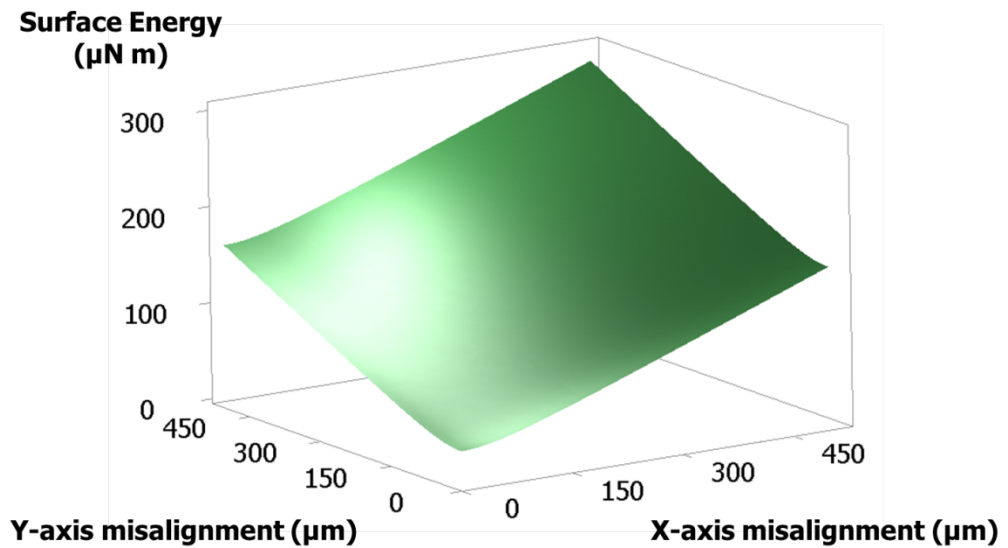


Figure 6-7: Surface plot of surface energy for combined lateral component misalignment in the x and y axes for 250 nl liquid volume.

The surface energy of the system was plotted against the combined lateral component misalignment in x and y axes (Figure 6-7 and Figure 6-8) for 250 nl liquid volume. From the data presented in Figure 6-8 it can be seen that for small component misalignments $<100 \mu\text{m}$ (as those experimentally investigated in Chapter 5, section 5.3), that the surface energy response is linear. This can be seen from the circular profile observed in the contour plot in Figure 6-8 b). As surface energy is linearly proportional to displacement,

the contribution of the misalignments in the x axis and y axis can be summed in quadrature, and displacements less than 100 μm can reasonably be represented by displacement magnitude.

As the component misalignment increases however, the response becomes non-linear and therefore caution must be used if considering large misalignments $>100\ \mu\text{m}$.

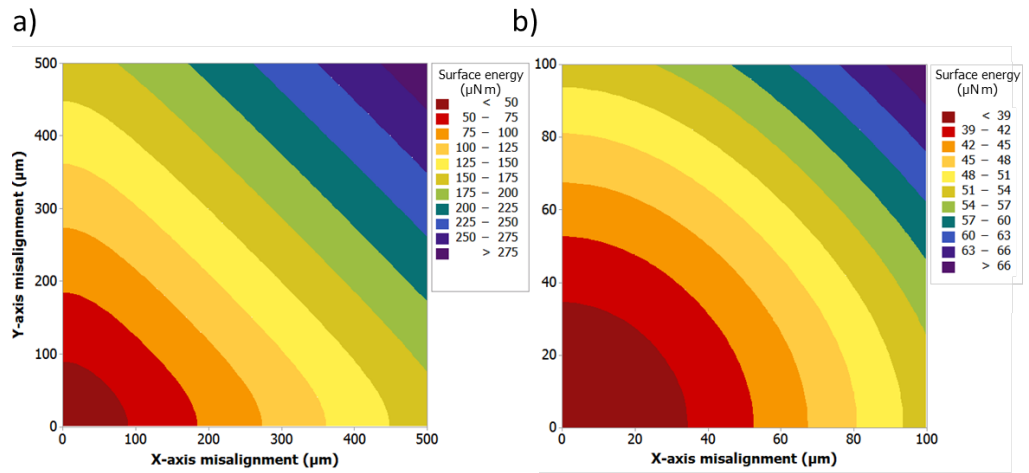


Figure 6-8: Contour plot of surface energy against component misalignment for the case of combined lateral misalignment in x and y axes for 250 nl liquid volume. a) 500 μm misalignment, b) 100 μm misalignment.

Plotting the data for 1000 nl liquid volume (Figure 6-9 & Figure 6-10), it can be seen that the surface energy is higher than that observed for 250 nl liquid volume. This is intuitive as the area of the liquid interface has increased with the increase in liquid volume. It can also be observed that the surface energy of the system is less affected by the component offset, with a linear response observed over higher component misalignments.

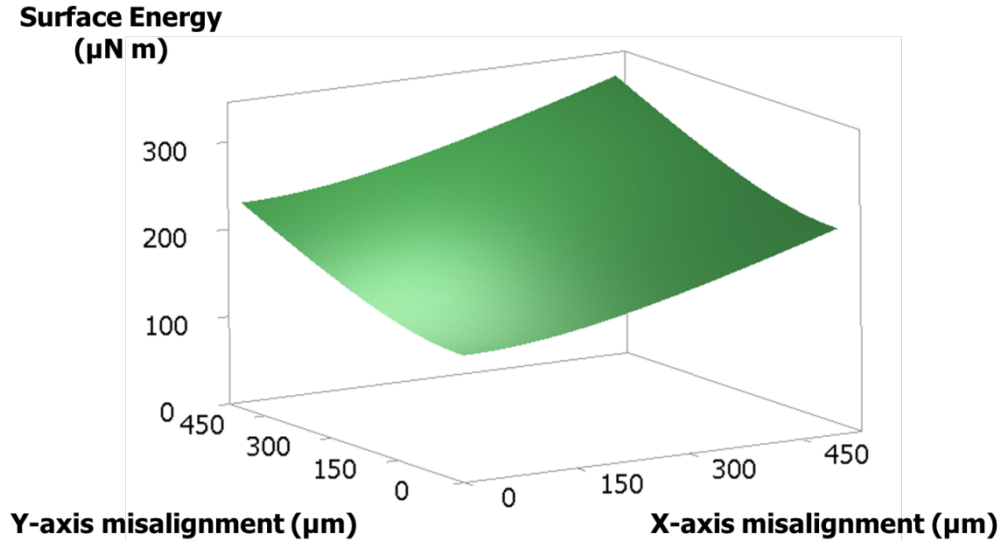


Figure 6-9: Surface plot of surface energy for combined lateral component misalignment in the x and y axes for 1000 nl liquid volume

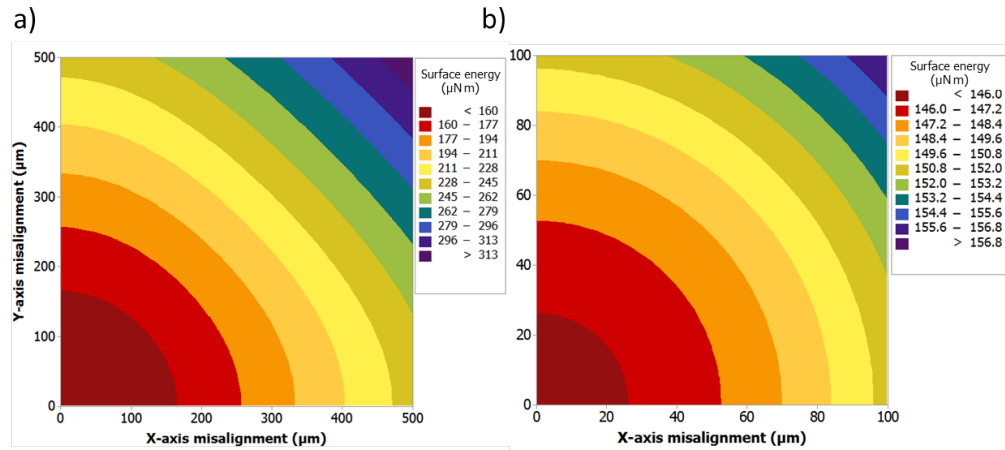


Figure 6-10: Contour plot of surface energy against component misalignment for the case of combined lateral misalignment in x and y axes for 1000 nl liquid volume. a) 500 μm misalignment, b) 100 μm misalignment.

6.4 Vertical displacement

This Surface Evolver simulation measures the stiffness characteristics of a liquid droplet undergoing component displacement in the z-axis. For a given liquid volume the system will have an equilibrium position where the weight of the component is equal to the capillary forces. When the component starts below the equilibrium position the liquid droplet is in compression causing the liquid to bulge out of the binding site, increasing surface area and therefore

surface energy. Conversely when the component is positioned above the equilibrium position the liquid droplet is in tension creating a concave surface and again increasing surface energy. The three states of compression, equilibrium and tension can be seen in Figure 6-11. The equilibrium point is therefore a balance between the gravitational and capillary forces. This is of particular interest to microassembly applications as the restoring force generated in the z-axis determines the maximum weight of component that can be placed on the liquid droplet without causing it to overflow the binding site. As was shown in the experimental investigation conducted in chapter 5, section 5.3, the containment of the liquid droplet on the binding site is extremely important as any overflow leads to systematic misalignment of the component. Additionally the determination of the restoring force in the z-axis can be applied in the context of a microhandling operation where a capillary gripper is used to pick-up and manipulate the component (see chapter 2, section 2.2.1 for an overview of capillary gripping). In this case the restoring force determines the maximum weight of component that can be picked up, or the surface interaction forces which need to be overcome to lift the component from its current position.

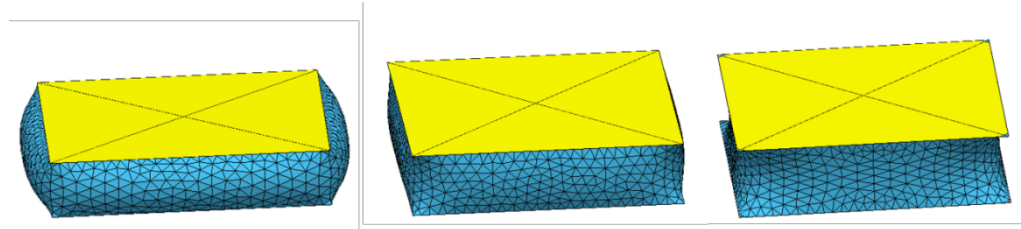


Figure 6-11: Rendered image of Surface Evolver model for the case of vertical displacement. (Left) Component while under an initial compression, (Centre) Fully assembled component in equilibrium position, (Right) Component while under an initial tension.

In this series of simulations three liquid volumes were examined: 250, 500 and 1000 nl. The equilibrium position of the component, h_0 , was determined by dividing the liquid volume by the cross-sectional area of the binding site top surface. The three equilibrium positions were 62.5, 125, and 250 μm above the binding site surface, for 250, 500 and 1000 nl liquid volumes respectively. The component was simulated either side of the equilibrium position by

displacement in the z-axis in 0.1 μm increments. This allowed the resolved lowest surface energy condition for each misalignment position to be determined.

Data files were generated by writing a batch script in Matlab which altered the component position in the x-axis by modifying the *zoffset* variable for each data file. Data files were then batch run in SE-FIT and their results extracted from the output file using a second Matlab script which identified the relevant lines.

The results were compared to a simple analytical solution based on a circular curvature of the interfaces. Analytical solutions for this case have been presented in two sources in the literature [9, 85], both of which contain errors in the derivation of the equation. A revised derivation of the analytical solution is presented in APPENDIX H.

The surface energy was plotted against misalignment position of the component for the three different liquid volumes. Due to the large differences in misalignment position for the three liquid volumes each was plotted separately for clarity (Figure 6-12 - Figure 6-14). Solid lines represent the numerical solution calculated in Surface Evolver, and dotted lines represent the analytical solution.

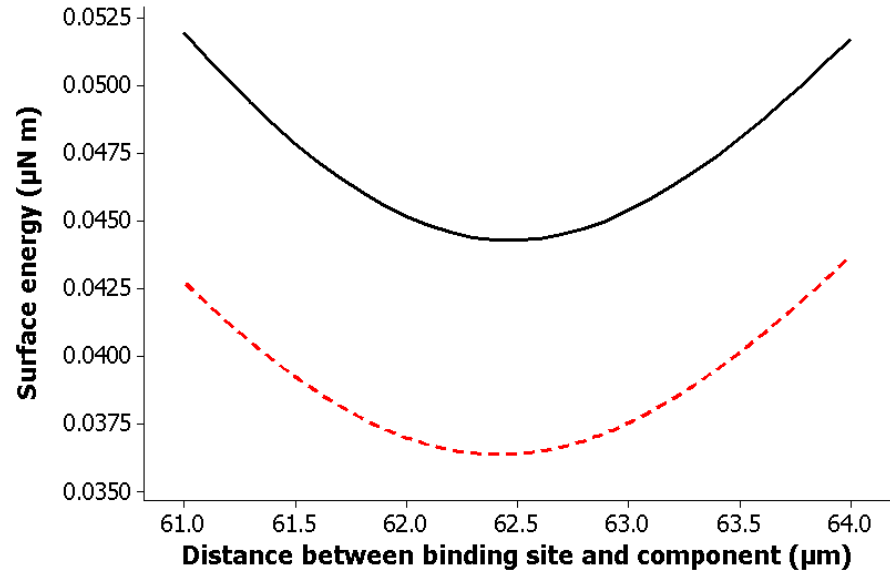


Figure 6-12: Plot of surface energy against distance between binding site and component for 250 nl liquid volume. Solid line shows Surface Evolver numerical solution, dotted line shows analytical solution.

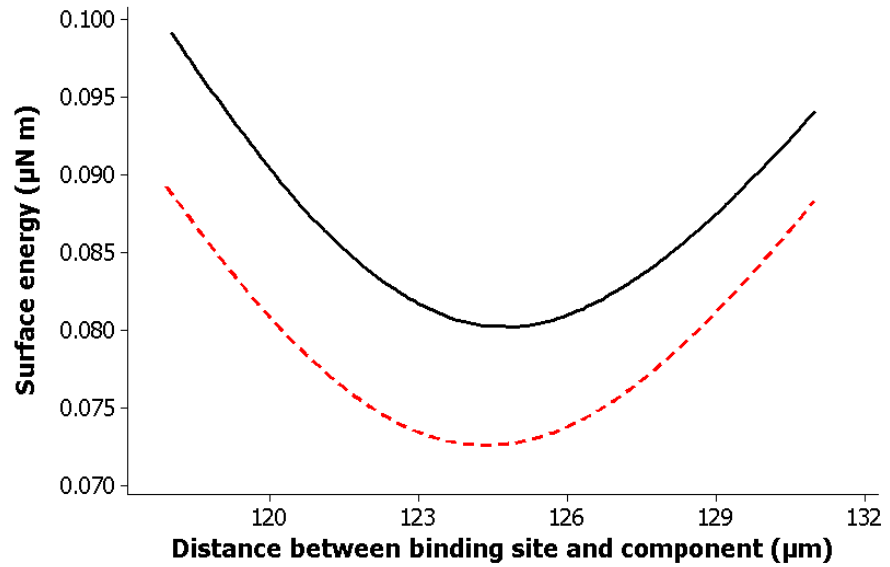


Figure 6-13: Plot of surface energy against distance between binding site and component for 500 nl liquid volume. Solid line shows Surface Evolver numerical solution, dotted line shows analytical solution.

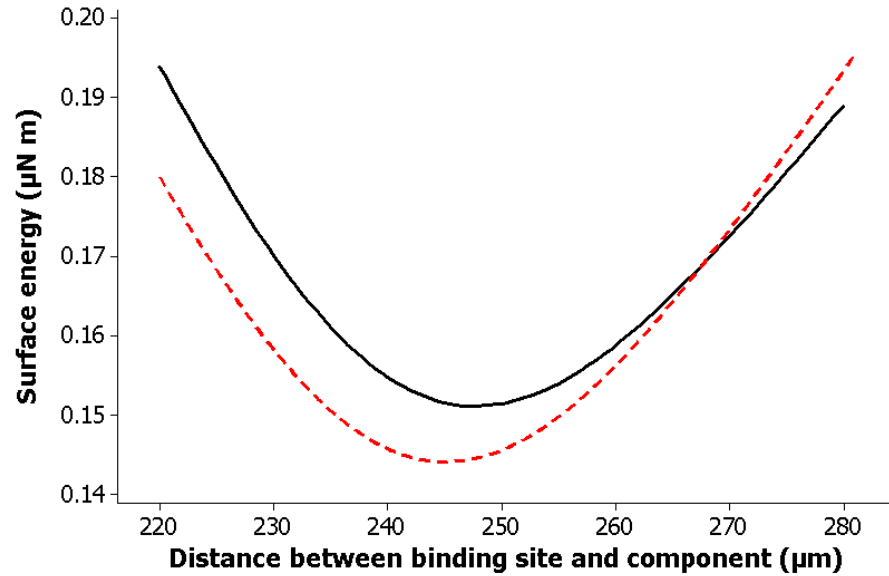


Figure 6-14: Plot of surface energy against distance between binding site and component for 1000 nl liquid volume. Solid line shows Surface Evolver numerical solution, dotted line shows analytical solution.

From the data it can be seen that each plot has a point of minimum surface energy located at the equilibrium position. Either side of this the surface energy rises due to distortions in the liquid droplet. As the distance between binding site and component is reduced the surface energy rises due to the liquid droplet being compressed. As the distance increases, surface energy also rises due to the droplet being stretched in tension. Once again it can be seen that higher surface energy values are obtained for larger liquid droplet volumes. It should be noted that the range of acceptable component positions is much smaller for lower liquid volumes compared to higher liquid volumes. At 250 nl liquid volume (Figure 6-12) the range is $\sim 4 \mu\text{m}$, whereas at 1000 nl liquid volume (Figure 6-14) the range is $\sim 60 \mu\text{m}$. The validity of the data obtained from Surface Evolver is heavily dependent on the user's ability to apply suitable physical limits to the model. As previously discussed, the software is simply trying to evolve the surface to a state of minimum surface energy. The software cannot detect if the model has entered a non-physical configuration, and may identify a minimum surface energy state which is impossible to achieve in reality. The user must therefore pay close attention to the model to ensure it is running correctly. If the distance between component and binding

site is reduced too much the liquid droplet bulges out in an unrealistic manner producing numerical errors, identifying a non-physical minimum energy state. (Figure 6-15). This observed bulging effect of the liquid would not be a valid physical condition as the droplet would have overflowed the binding site, resulting in failed alignment of the component. The limitation in the range of valid component positions is due to model simplification which assumes that the liquid remains pinned along the binding site and component edges.

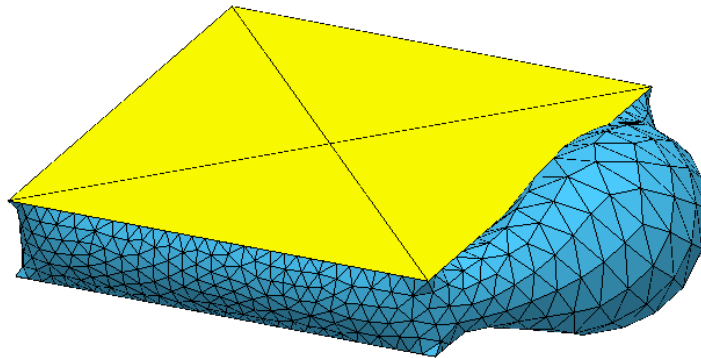


Figure 6-15: Surface evolver model illustrating the bulging effect when compressing the assembly liquid beyond a certain point for a given liquid volume.

Data were imported into Matlab where a numerical differentiation was performed using a spline fit to obtain the force exerted by the liquid droplet on the component. Data were then smoothed by fitting a 6th order polynomial. The restoring force was plotted as an absolute value, i.e. compressive and tensile forces were plotted as positive for clarity and ease of comparison. Once again data for each liquid droplet volume was plotted separately due to the vast difference in range of component positions (Figure 6-16 - Figure 6-18).

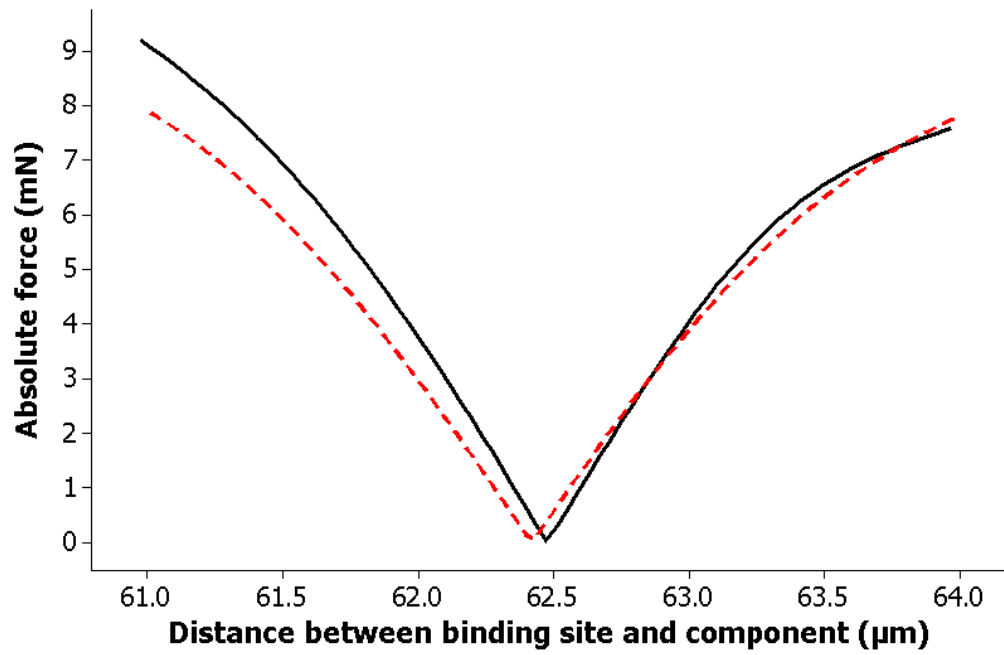


Figure 6-16: Plot of absolute force against distance between binding site and component for 250 nl liquid volume. Solid line shows Surface Evolver numerical solution, dotted line shows analytical solution.

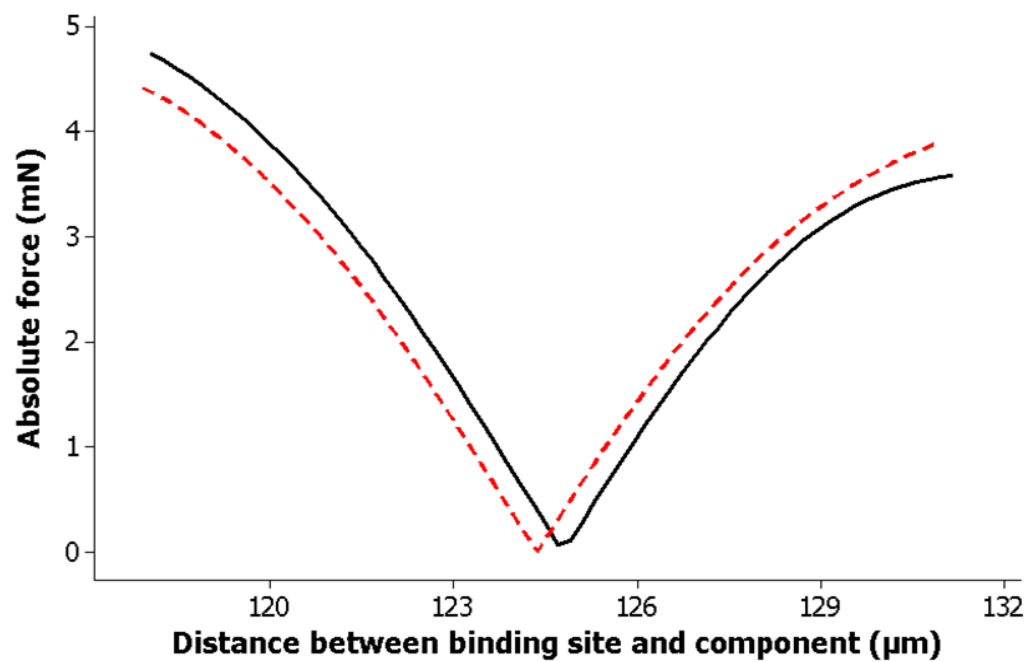


Figure 6-17: Plot of absolute force against distance between binding site and component for 500 nl liquid volume. Solid line shows Surface Evolver numerical solution, dotted line shows analytical solution.

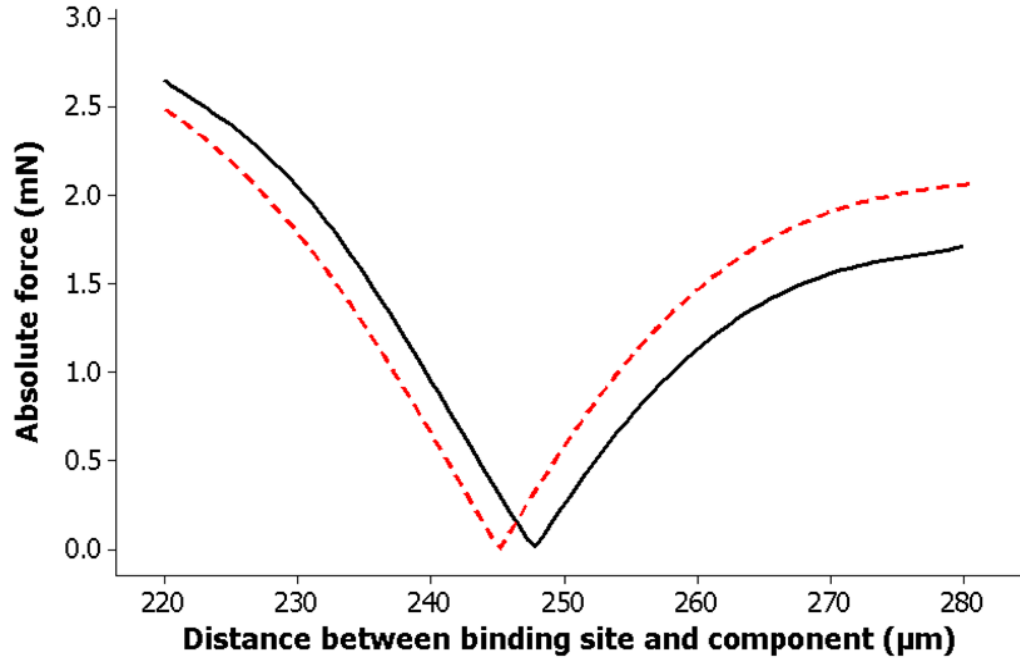


Figure 6-18: Plot of absolute force against distance between binding site and component for 1000 nl liquid volume. Solid line shows Surface Evolver numerical solution, dotted line shows analytical solution.

The data reveal that higher restoring force is obtained at smaller liquid volumes. It can also be seen that the force is applied over considerably smaller distances of component misalignment about the equilibrium position for smaller liquid volumes. This indicates that a much stiffer response is obtained when smaller liquid volumes are used. This is useful for microdroplet alignment applications as it shows that heavier components can be assembled when the liquid volume is small. It also suggests that for microhandling applications use of low liquid volumes increases the mass of component which can be picked up and manipulated.

In chapter 5, section 5.4 square binding sites of 1.75 x 1.75 x 0.1 mm were experimentally investigated using a nanoindenter. The process of probing the liquid droplet with the modified nanoindenter tip is similar to the numerical modelling of the vertical displacement case presented in this section. It is important to note however that there are some key differences between the two, and therefore should in no way be considered a validation. Firstly the experimental square binding sites are different dimensions, with the numerical

model being 2 x 2 x 0.1 mm. Secondly the numerical solution assumes complete wetting of both the binding site and component and that the liquid droplet remains pinned to the edges. Considering the profile of the data produced in chapter 5, section 5.4 it is possible to compare events in the droplet behaviour to those observed during numerical simulation (Figure 6-16 - Figure 6-18). The tension phase (above component equilibrium position) cannot really be compared due to the conditions being very different. It is possible to observe a point of inflection however where the component (or indenter tip) passes through the equilibrium position and then continues to compress the liquid droplet which can be seen by an increase in force. Comparing the data sets it can be seen that the forces recorded during the nanoindenter testing are of a comparable magnitude and scale to the numerical solution. Maximum forces observed during the experimental investigation were ~3 - 5 mN for liquid droplet volumes of 267 – 365 nl. This is compared to simulated maximum forces of ~2.5 – 9 mN for liquid droplet volumes of 250 – 1000 nl.

6.5 Torsional displacement

This Surface Evolver simulation measures the rotational stiffness characteristics of a liquid droplet undergoing component displacement around the z-axis. The torsional coefficient is similar to that of Hooke's Law and is given by the equation:

$$\tau = -k\theta \quad (6-8)$$

A torsional displacement creates a distortion of the liquid droplet which leads to an increase in surface energy. The restoring torque exerted by the liquid droplet to bring the component equilibrium can be found by the differential of the surface energy with respect to the angular misalignment of the component:

$$T = \frac{\delta(\gamma S)}{\delta\theta} \quad (6-9)$$

Where γ is surface tension, S is the interfacial area, and θ is the component rotational misalignment about the z-axis.

In this series of simulations three liquid volumes were examined: 250, 500 and 1000 nl. The displacement of the component was simulated from zero rotational misalignment i.e. perfectly aligned with the binding site, to 45° misalignment around the z-axis in 0.5° increments (Figure 6-19). This allowed the resolved lowest surface energy condition for each misalignment position to be determined.

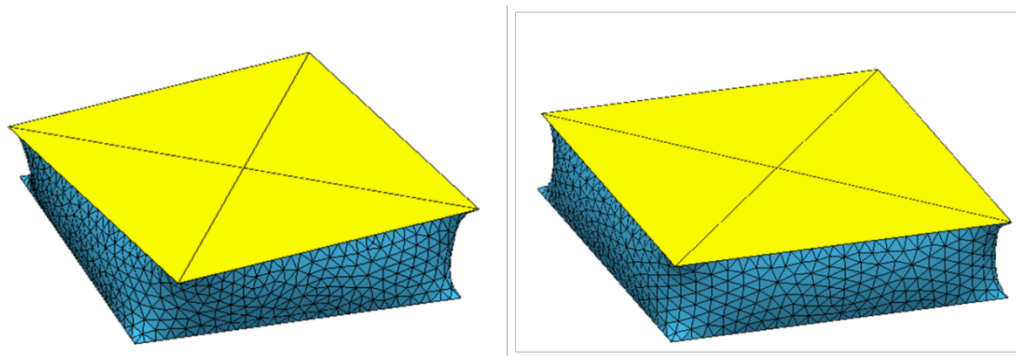


Figure 6-19: Rendered image of Surface Evolver model for the case of torsional displacement. (Left) Component with an initial rotational misalignment of 10 degrees. (Right) Fully assembled component in equilibrium position.

Data files were generated by writing a batch script in Matlab which altered the component position around the z-axis by modifying the *yaw* variable for each data file. Data files were then batch run in SE-FIT and their results extracted from the output file using a second Matlab script which identified the relevant lines.

The surface energy of the liquid-air interface can be shown to be [85]:

$$E = 4\gamma \left[sh\sqrt{1+a^2} + \frac{h^2}{\theta} \ln \left(a + \sqrt{1+a^2} \right) \right] \quad (6-10)$$

Where $a = s\theta/h$, $s = L/2$, L is length of component edge, γ is surface tension, h is the distance between the binding site surface and component, and θ is the angle of rotation in radians.

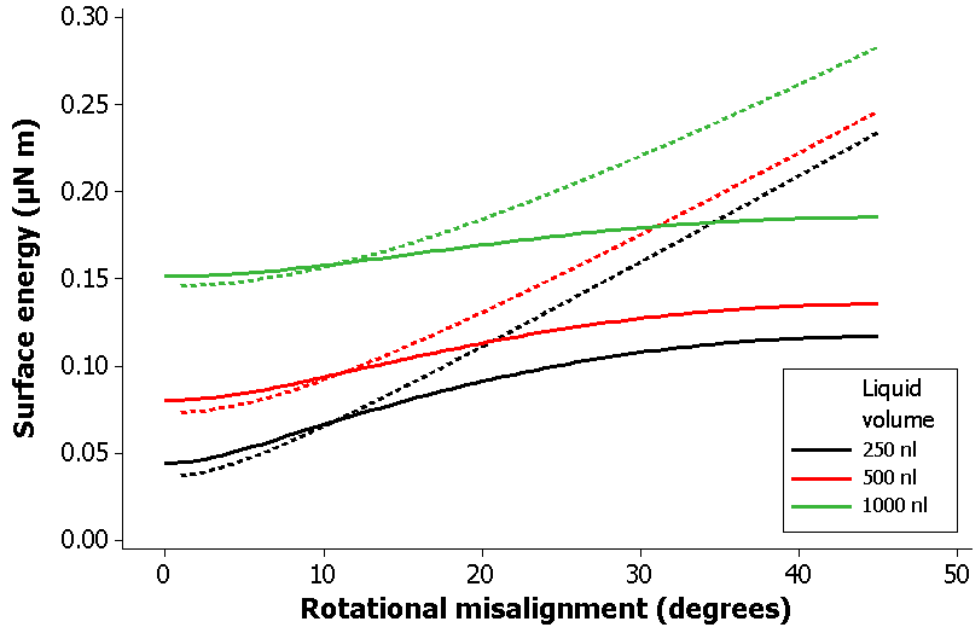


Figure 6-20: Plot of surface energy against component rotational misalignment for varying liquid volume. Solid lines show Surface Evolver numerical solution, dotted lines show analytical solution.

From Figure 6-20 it can be seen that the analytical solution agrees reasonably well with the Surface Evolver derived numerical solution for the first 15° of misalignment. After this point the results differ significantly due the simplification of the analytical solution which does not represent the actual physical shape of the surface well at large rotational angles.

Data were imported into Matlab where a numerical differentiation was performed using a spline fit to obtain the restoring torque exerted by the liquid droplet on the component. Data were then smoothed by fitting a 6th order polynomial. The restoring torque was compared to a simple analytical solution (Equation (6-11)) [85] with restoring torque plotted against angle of rotation of the component (Figure 6-21).

$$T \approx \gamma L^2 \left[\frac{a}{\sqrt{1+a^2}} + \frac{1}{a + \sqrt{1+a^2}} \left(\frac{1}{a} + \frac{1}{\sqrt{1+a^2}} \right) - \frac{\ln(a + \sqrt{1+a^2})}{a^2} \right] \quad (6-11)$$

Where $a = L\theta/2h$, γ is surface tension, L is the length of component edge.

Figure 6-21 shows that the restoring torque obtained from the analytical solution does not agree well with the results from Surface Evolver for the case of rotational misalignment of the component. Consider the rotation of a square component about the z-axis (Figure 6-22). At 45° misalignment a corner of the component (marked in the diagram by a red dot) is directly between two positions of minimum energy. At 45° misalignment the liquid droplet is at its most distorted, meaning surface energy is at its maximum. Rotation of the component in either direction will result in a reduction in surface energy. This means that there will be a saddle point at 45° misalignment which when differentiated will result in zero restoring torque. This indicates that the numerical solution obtained from Surface Evolver is a much more realistic representation of the physical behaviour of a component during rotational misalignment than the analytical solution. The data show that higher restoring torque is obtained at lower liquid volumes. The data also reveal that the rate at which the maximum restoring torque is reached is much faster for lower liquid volumes shown by the gradient of the data line and indicating a stiffer response. Additionally, the maximum torque occurs at lower angles of rotational misalignment of the component for lower liquid volumes. These observations are particularly useful for component alignment applications as they could for example be applied to a situation where rather than assembling a misaligned component, the liquid droplet is used to provide torsional resistance to prevent axial component rotation.

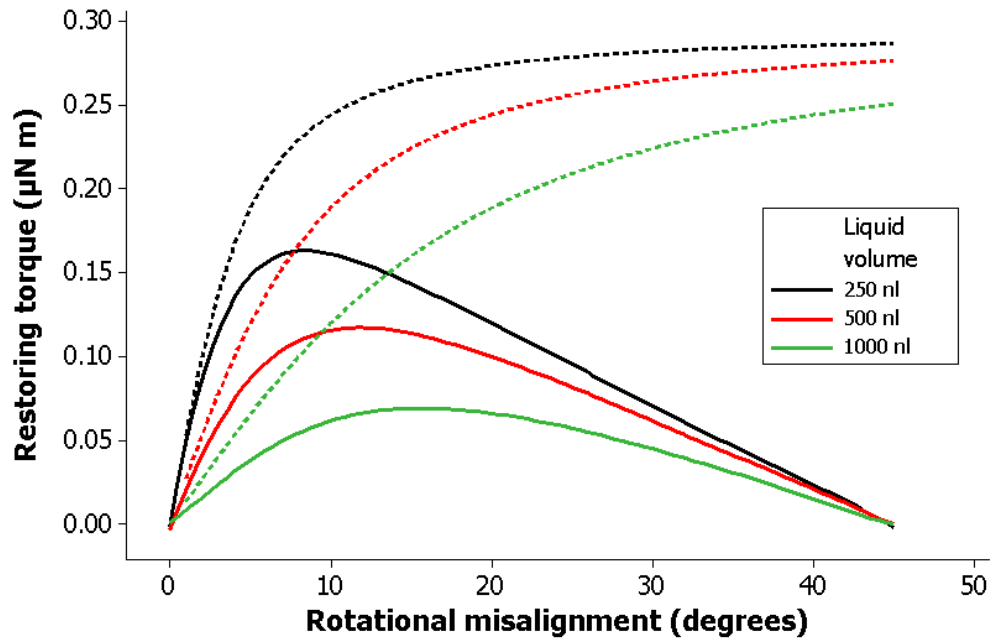


Figure 6-21: Plot of restoring torque against component rotational misalignment for varying liquid volume. Solid lines show Surface Evolver numerical solution, dotted lines show analytical solution.

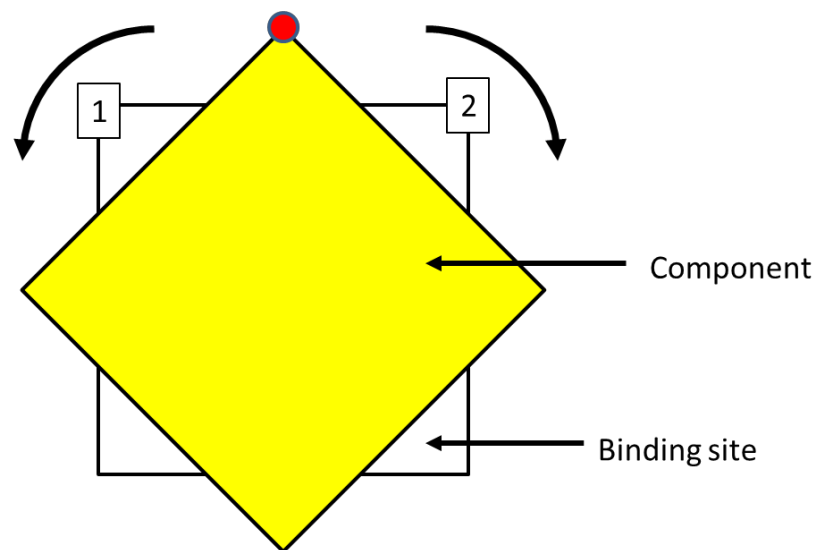


Figure 6-22: Diagram showing the rotation of a component at 45 misalignment. The corner signified by the red dot can obtain a minimum energy position by rotating to either position 1 or 2.

6.6 Tipping displacement

This Surface Evolver simulation measures the tipping stiffness characteristic of a liquid droplet undergoing component displacement around the x, or y-axes

In this series of simulations three liquid volumes were examined: 250, 500 and 1000 nl. The displacement of the component was simulated from zero misalignment i.e. perfectly aligned with the binding site, to 3.2° displacement around the x-axis for 250 nl liquid volume, 5.7° for 500 nl liquid volume and 10° for 1000 nl liquid volume, in 0.1° increments (Figure 6-23). This allowed the resolved lowest surface energy condition for each misalignment position to be determined.

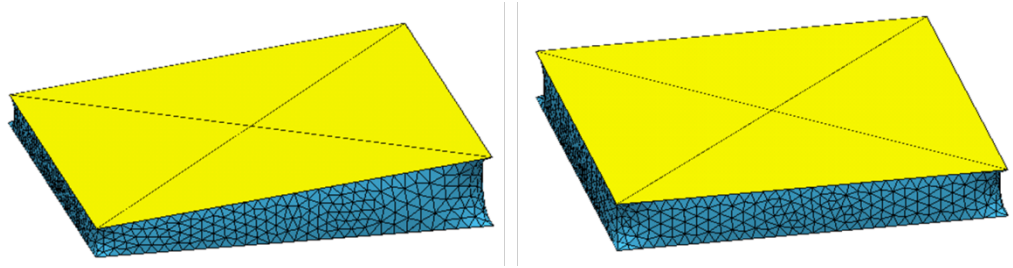


Figure 6-23: Rendered image of Surface Evolver model for the case of tipping displacement. (Left) Component with an initial tipping misalignment of 6 degrees. (Right) Fully assembled component in equilibrium position.

Due to the way the model is constructed the component tipping position occurs about the central coordinate system as illustrated in Figure 6-24. This results in the component passing through the geometry of the binding site at larger tipping angles. This is an unphysical situation which results in inconsistent changes in surface energy relative to component tipping position. This means that the model is only valid for simulating a small range of component tipping angles, and justifies why different ranges of tipping angle were required for the three different simulated liquid volumes in order to obtain meaningful results.

Data files were generated by writing a batch script in Matlab which altered the component tipping position around the x-axis by modifying the *roll* variable for each data file. Data files were then batch run in SE-FIT and their results

extracted from the output file using a second Matlab script which identified the relevant lines.

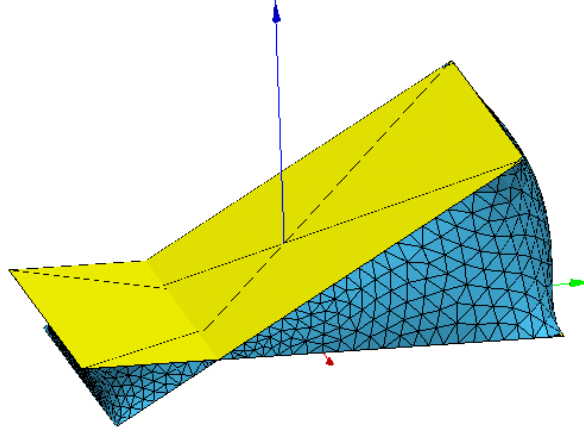


Figure 6-24: Rendered image of Surface Evolver model for the case of tipping displacement showing the issue that occurs when simulating large tipping angles.

The results were compared to a simple analytical solution which assumed the component surface energy while in its equilibrium position above the binding site [85]:

$$E = \gamma S = \gamma(4Lh) \quad (6-12)$$

Where γ is surface tension, S is interfacial area, L is the length of component edge, and h is distance between binding site top surface and component.

The surface energy was plotted against tipping misalignment of the component about the x-axis for the three different liquid volumes (Figure 6-25). Solid lines represent the numerical solution calculated in Surface Evolver, and dotted lines represent the analytical solution obtained from equation (6-12). From the data it can be seen that the surface energy varies extremely slowly for component tipping misalignment around the x-axis, with numerical results obtained from Surface Evolver being very similar to that of the analytical approximation for a component in equilibrium. This result is intuitive when considering that a rotation about the x-axis when the coordinate system is central will result in a slight compression of the liquid droplet on one side, and

a slight tension of the liquid droplet on the other. The relative distortion of the liquid droplet will not change significantly, meaning the change in surface area will therefore be small, hence a small change in the surface energy. Again it can be observed that higher surface energy is obtained for a larger liquid volume.

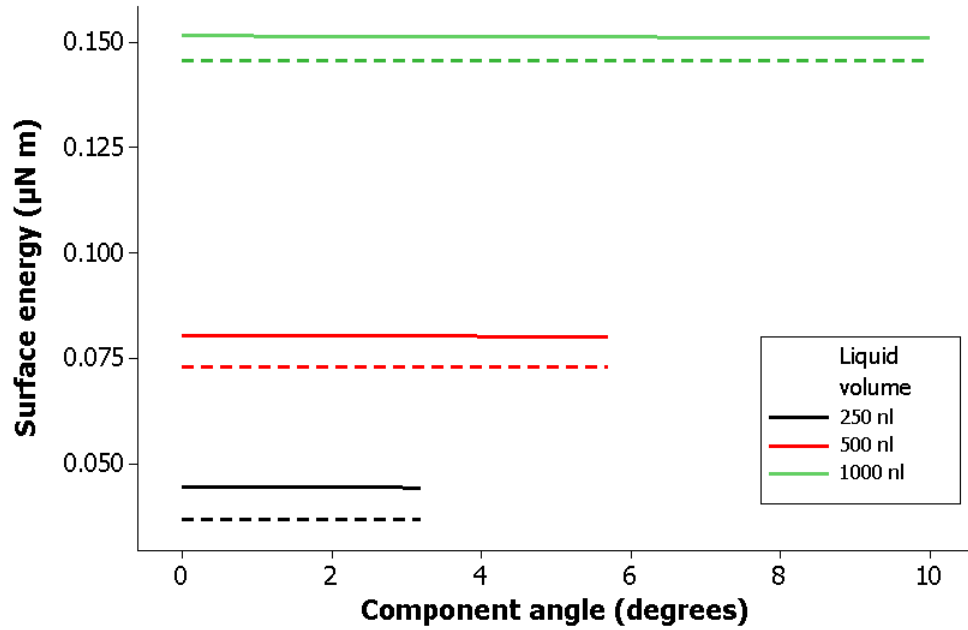


Figure 6-25: Plot of surface energy against component tipping misalignment around the x-axis for varying liquid volume. Solid lines show Surface Evolver numerical solution, dotted lines show analytical solution.

As for the previous degrees of freedom, the force exerted on the component is found from the differential of the surface energy with respect to the change in component position (equation (6-13)). A numerical differentiation of the surface energy was not appropriate in this case however due to the very small change in surface energy as component angle increased.

$$T = \frac{\delta(\gamma S)}{\delta\theta} \quad (6-13)$$

From this observation it can be concluded that the restoring torque produced by the liquid droplet for this degree of freedom must be very small compared to the other DOF.

The low restoring torque about the x-axis indicates that the component is likely to tip about this axis and make contact with the binding site when placed on the liquid droplet. This will be more apparent at higher liquid volumes as the response is less stiff than at lower liquid volumes. It was shown above in Figure 6-24 that this particular model is unable to simulate the liquid droplet behaviour at large misalignment angles due to the component passing through the binding site geometry. A new model will be created to address this scenario and investigate the ability to provide vertical component alignment. This work will be presented in Chapter 8 along with a numerical solution and experimental investigation. Additionally the Surface Evolver derived spring constant will be integrated in a commercially available CAE package to demonstrate how the liquid droplet behaviour can be applied in a design environment.

6.7 Summary

This chapter presented the use of the Surface Evolver software to numerically model the self-alignment of micro components using liquid surface tension. Surface Evolver is free-to-use software designed to simulate the behaviour of surfaces shaped by surface tension and other forces.

A series of simulations were presented which considered the alignment of a component onto matching binding sites. A simulation was conducted for each degree of freedom (DOF) to isolate the forces exerted on the component by a liquid droplet and how this may influence alignment. The misalignment cases investigated were lateral component misalignment in the x or y-axes, vertical component misalignment in the z-axis, torsional component misalignment about the z-axis, and tipping displacement about the x or y-axes. The purpose of these simulations was to establish a set of spring constants which could later be integrated into a more complex computer aided engineering (CAE) design study presented in chapter 8.

Across all simulations higher surface energy was observed for larger liquid volumes due to the increase in liquid surface area. It was also seen that higher

restoring forces as well as stiffer responses were observed for smaller liquid volumes due to the relative distortion in liquid droplet shape for a given component misalignment. Results from each simulation were compared to a simple analytical solution. In general the numerical and analytical solutions compared well, with Surface Evolver numerical solutions tending to produce a slightly higher surface energy result due to the shape of the interface adopting a minimal surface.

The lateral displacement case showed good agreement between analytical and numerical solutions for component misalignment up to 0.5 mm. Restoring force was shown to remain constant after reaching a maximum for increasing component misalignment indicating strong liquid droplet alignment capabilities for this degree of freedom.

Numerical data for the case of vertical displacement showed good agreement with the analytical solution. Comparisons were made between the vertical displacement case and the experimental investigation using the nanoindenter in chapter 5, section 5.4. It was stressed that data should not be treated as a validation due to distinct differences between the two cases. Restoring forces obtained from the experimental and numerical work were of a similar order of magnitude and range. Maximum forces observed during the experimental investigation were ~3 - 5 mN for liquid droplet volumes of 267 – 365 nl, compared to Surface Evolver simulated maximum forces of ~2.5 – 9 mN for liquid droplet volumes of 250 – 1000 nl.

For the case of torsional displacement the analytical solution did not compare well to the simulated results at larger rotational angles. This was due to the significant difference in shape of the liquid droplet between the two solutions. It was shown that the analytical solution did not reasonably represent the droplet shape at large rotational angles and therefore was not comparable to the minimum surface produced using Surface Evolver.

In the case of tipping misalignment about the x or y-axes it was noted that the change in surface energy with respect to component angle was extremely

small. This meant it was not appropriate to conduct a numerical differentiation to obtain the restoring torque. It was concluded that the restoring torque offered by the liquid droplet in this DOF was extremely small and would lead to the component touching down on one edge of the binding site. Additionally the model was noted to be inadequate for simulating large angles of misalignment during the tipping simulations due to the component passing through the binding site geometry and creating an unphysical condition.

This work has shown that Surface Evolver works well for simple geometries, showing good agreement with simple analytical solutions and capable of predicting comparable forces for some experimental cases previously investigated in the thesis. For complex geometries however or when iterative design decisions are necessary, Surface Evolver becomes inadequate, and the work would want to be carried out in a more flexible CAE package which allows optimisations to be performed.

In the next chapter the use of Surface Evolver for modelling the effect of non-idealised binding site edge geometries is presented. This work is intended to investigate the effect non-idealised binding sites on the surface energy of liquid droplets during the alignment process, thus addressing the project objective.

Chapter 7

7 MODELLING THE EFFECT OF EDGE GEOMETRY ON LIQUID DROPLETS USING SURFACE EVOVLER

This chapter considers the effect of non-sharp edges, and undercut features on the binding sites used to constrain liquid droplets. The work will focus on the effect these features have on liquid droplets when being used for micro component assembly tasks. This work is conducted using the free-to-use software Surface Evolver. The previous model presented in section 6 for the determination of spring constants, as well as other models presented in the literature assumed that the assembly liquid had fully wetted both the binding site and component and was pinned along their edges. The Gibbs inequality (chapter 2, section 2.4.12) also assumes that structures have a mathematically sharp edge at the intersection between the sidewall and binding site top surface. In reality however a perfectly sharp edge is unachievable regardless of the manufacturing process and these existing models therefore represent a highly idealised case. Indeed, the experimental work presented in chapter 5 showed that components produced on the EnvisionTec Perfactory exhibit a strong radius edge which is believed to affect the structures ability to pin the triple contact line (TCL) of the liquid droplet. It is proposed that the surface energy penalty for a liquid moving around a curved edge will be significantly lower than that of a perfectly sharp edge and will be proportional to the radius of the edge. This means that it would be easier for a liquid droplet to overflow a binding site with a large radius at its edge.

The work presented in chapter 5 also revealed that the undercut edge geometry of the binding site played a significant role in the structures ability to constrain liquid spreading, as well as its capacity to provide alignment for micro components using liquid surface tension. It was found that much higher contact angles, as well as superior alignment results were obtained when the edge geometry was undercut with angles $<90^\circ$, compared to binding sites whose edge geometry was $>90^\circ$. Cross sectional analysis of the fabricated components however revealed that the manufacturing process failed to faithfully recreate the desired edge geometry making it difficult to quantify the

role these features played. Surface Evolver's ability to model the effect of binding site undercut on surface energy of the system will be investigated in section 7.2.

The experimental work presented in chapter 5 revealed some interesting observations relating to the binding site structures ability to control liquid spreading and offer accurate and repeatable micro component alignment. Due to limitations in the experimental setup such as the inability to control the edge radius of the binding sites, and imprecise control of the applied liquid volume, means an investigation of these factors via purely experimental means would be difficult without collecting a substantial data set. The use of Surface Evolver allows a detailed analysis of a large range of parameters through numerical modelling of the system, allowing comparisons to be drawn against the previously observed experimental behaviour.

7.1 Modelling curved edges

Previous models that address micro component alignment presented in the literature have always simplified the physical geometry of the system and assumed that the liquid remains entirely on the binding site. These models have not attempted to account for variations in the profile of the binding site edge. In these previously presented models, the liquid position is pinned along the perimeter of the binding site which effectively models an infinitely sharp edge. As was shown in chapter 5, physical structures display a radius along their edges, the extent of which will be determined by the manufacturing process. It is proposed that the radius at the edge of the binding site reduces the structures ability to control liquid spreading, and is also detrimental to the structures capacity to offer accurate and repeatable self-alignment using liquid surface tension. The work presented in this section models the effect of edge radius on the surface energy of the system when the assembly liquid is allowed to move from the idealised state on the binding site top surface, along the curved edge and down the binding site sidewall.

The model presented in this section was designed to represent the physical geometries which were created in this thesis using the EnvisionTec Perfactory. Square binding sites of dimensions $2 \times 2 \times 0.1$ mm, along with matching components of $2 \times 2 \times 0.5$ mm, and an assembly liquid of water (Figure 7-1) were used.

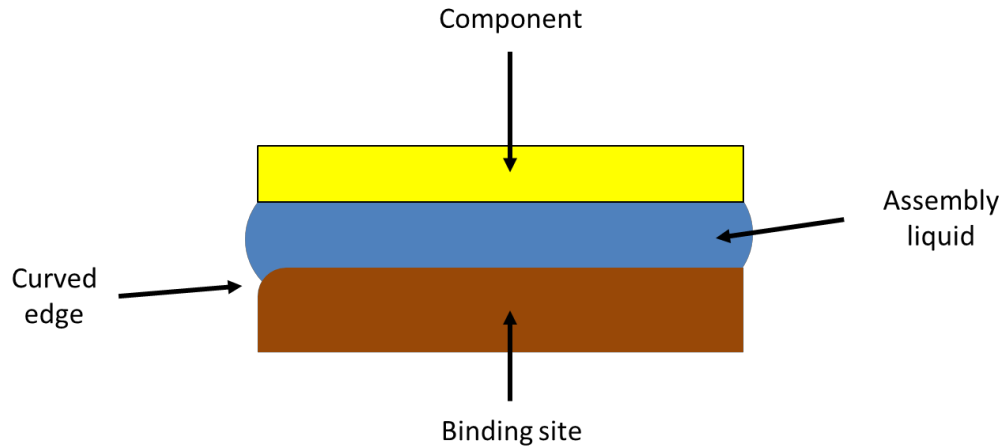


Figure 7-1: Cross-sectional diagram illustrating the setup of the model.

It was assumed that the vertical sidewalls retain the major component dimensions of 2×2 mm, and that the top surface of the binding site is $100 \mu\text{m}$ high. The radius was assumed to be uniform, and follow the perimeter of one edge of the top of the binding site (Figure 7-2). The component was assumed to retain its sharp edges and was fully wetted with the liquid pinned along its perimeter.

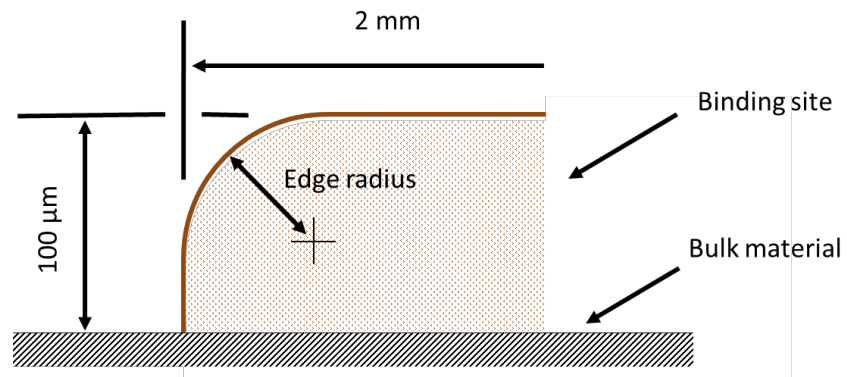


Figure 7-2: Cross-sectional diagram detailing the definition of the binding site.

Initially the model was created with the radius edge geometry applied to all four sides of the square binding site. This approach however resulted in errors occurring during simulation whereby the liquid droplet evolved into unphysical shapes (Figure 7-3). This was believed to be caused by a conflict occurring at the intersection of two circular edge constraints which made the liquid droplet vertices placed on these constraints behave in an unphysical way. At present the authors were unable to find a solution to this challenge and it was chosen to simplify the modelling approach to investigate the effect of only a single curved edge. The model data file can be found in APPENDIX I.

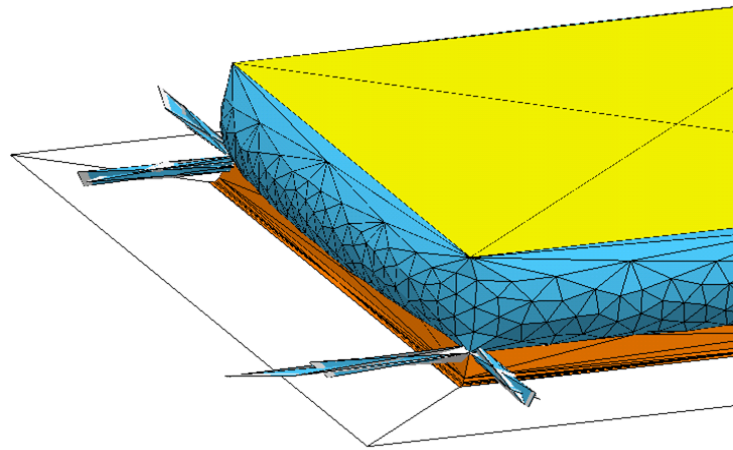


Figure 7-3: Rendered image of Surface Evolver model showing error which occurs during simulation of curved edges when applied to all four edges of a square binding site.

The different edge radii investigated in this section were an infinitely sharp edge with no radius, 5 μm radius, 25 μm radius, and 50 μm radius. These are illustrated in Figure 7-4 with dashed lines representing the original sharp edge geometry with no radius. Liquid droplet volumes of 345 – 365 nl in 5 nl increments were simulated. For each simulation the component position was held constant at 87.5 μm above the binding site top surface. This was determined by assuming a liquid volume of 350 nl, divided by the area of the binding site top surface. A fixed component position was selected and the liquid droplet volume altered to simulate the effect of the droplet being forced over the edge due to being over compressed. This would occur for example if the component was too heavy to be supported by the liquid droplet.

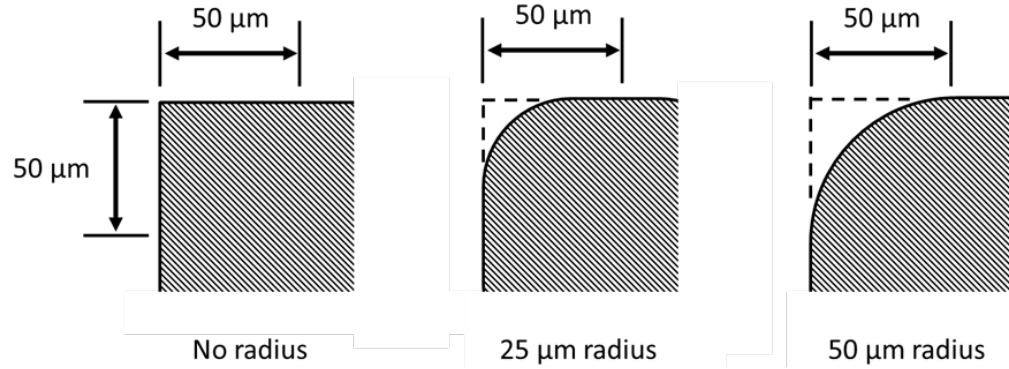


Figure 7-4: Cross-sectional diagram of curved edge geometry showing no radius, 25 μm radius, and 50 μm radius.

In order to model the radii of the edges in Surface Evolver a circle must be defined as a constraint and then the corresponding vertices, edges and facets placed on the constraint. A level-set constraint is used to fix vertices, edges of facets so that they may only exist at a location prescribed by an expression. The formula can contain any expression that is known to Surface Evolver or variables that have been previously declared in the data file. A full introduction to constraints within Surface Evolver can be found in APPENDIX C.

In order to investigate the effect of edge radius on the surface energy in the system a fixed liquid volume was moved through different fixed positions across the binding site top surface and sidewall. For each position the resolved minimum surface energy for each position was determined. When the binding site has an infinitely sharp edge the normal pinning position for the liquid, as in previous models presented in section 6, was to fully wet the binding site, with the droplet pinned along its perimeter. In the simulations presented in this section the pinning position for one edge of the liquid droplet was altered in 5 μm steps along the binding site top surface. The intersection between the binding site top surface and sidewall will be referred to as the zero position. The position of two vertices and their corresponding edge of the liquid droplet were moved in 5 μm steps along the binding site top surface up to 50 μm , which will be referred to as the range 0 to -50 μm . Depending on the simulated position of the liquid droplet, the base of the droplet will be in contact with

different parts of the binding site. For example in a simulation where the liquid droplet is positioned on the binding site top surface, then the droplet base is only in contact with the top surface and requires only a single facet. However, when the liquid droplet is simulated as having flowed over the sidewall the liquid droplet base is in contact with not only the binding site top surface, but also the curved edge and the sidewall. The droplet base then must be described using three facets to account for each of these areas. The challenge arises in that this cannot be achieved through a single model. To overcome this a model was created for each of the three pinning situations (top surface, curved edge, and sidewall) and the results then stitched together to produce a complete profile of the liquid droplet behaviour.

For liquid droplet positions on the sidewall a second model was created, and again the pinning position varied in 5 μm steps along the binding site sidewall down to 50 μm , which will be referred to as the range 0 to +50 μm . To increase the resolution of the models around the sharp corner, steps of 1 μm were used between the ranges of -5 to +5 μm . This is illustrated in Figure 7-5 a). In order to model the droplet pinning position along a curved edge a third model was required to account for the curved face. The droplet pinning position around the radius was altered in 5° increments, between the range of angles of 0 - 90°, with the vertices coordinates determined by calculating the corresponding arc length (Equation (7-1) and Figure 7-6). In the case of 25 μm edge radius, three models were used: the first for the binding site top surface covering the range of -25 to -50 μm in 5 μm increments, the second for the curved face covering the range of 0 - 90° in 5° increments, and the third for the binding site sidewall covering the range of 25 – 50 μm in 5 μm increments (Figure 7-5 b)). A similar approach was used in simulating a 5 μm edge radius, however the range on the binding site top surface and sidewall were -5 to -50 μm , and 5 to 50 μm respectively. In the case of 50 μm edge radius the full simulation could be performed using only the curved model as all pinning positions occurred around the radius edge.

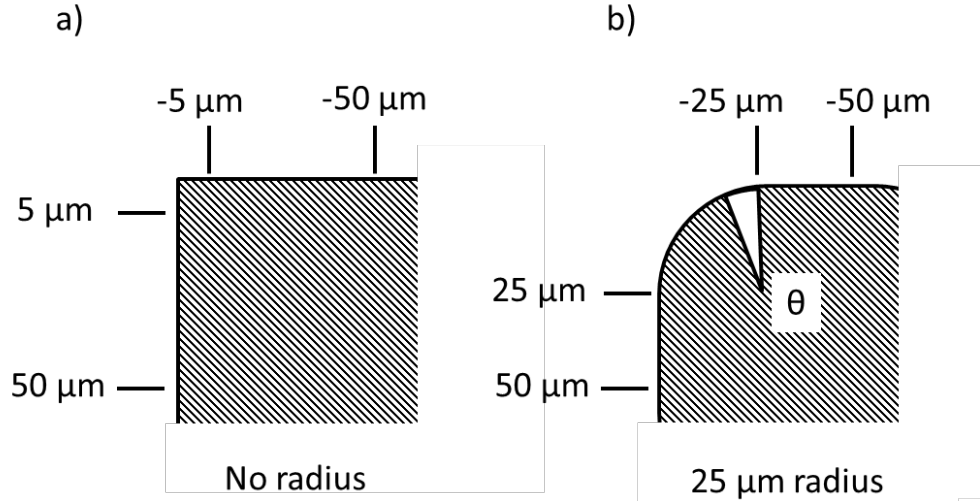


Figure 7-5: Cross-sectional diagram illustrating the pinning position of the liquid droplet at different positions on the binding site. a) binding site with sharp edge and no radius, b) binding site with 25 μm radius, θ is the segment angle which was 5° .

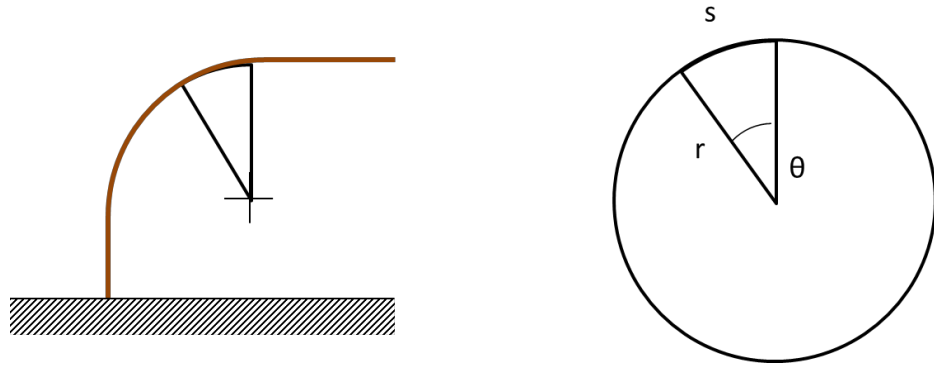


Figure 7-6: Diagram illustrating the calculation of droplet pinning position based on arc length.

$$\theta = \frac{s}{r} \quad (7-1)$$

Where θ is angle of arc in radians, r is radius of circle, s is arc length.

Screenshots of the three Surface Evolver models for the case of 25 μm radius are shown in Figure 7-7. These illustrate the droplet pinning position when on a) the binding site top surface, b) the curved 25 μm radius, and c) the binding site sidewall.

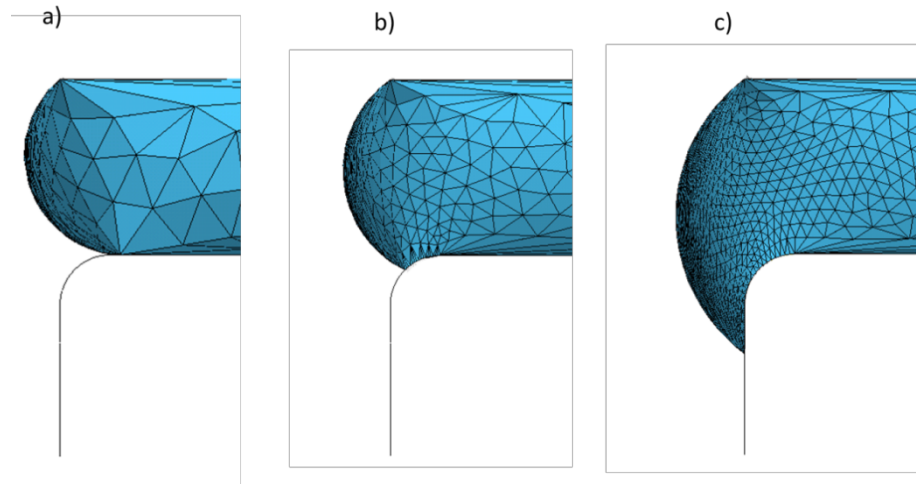


Figure 7-7: Close-up view of the three Surface evolver models for the case of 25 μm radius illustrating the different droplet pinning positions. a) binding site top surface, b) binding site radius, c) binding site sidewall.

Data files were generated by writing a batch script in Matlab which altered the liquid droplet pinning position along the binding site top surface, curved edge and binding site sidewall. Data files were then batch run in SE-FIT and their results extracted from the output file using a second Matlab script which identified the relevant lines. The data for each of the models were then stitched together to produce a full profile of the liquid droplet behaviour. Surface energy was plotted against pinning position for a liquid volume of 360 nl for the different edge geometries (Figure 7-8).

It can be seen that the lowest surface energy is obtained when the edge is infinitely sharp, with surface energy increasing as the edge radius is increased. The data also show that the lowest surface energy position was located at the intersection of the binding site top surface and sidewall for the infinitely sharp edge but moved progressively further around the curved edge as the radius increased. The implication of this observation to the alignment of components is extremely important. Component alignment is driven by the liquid droplet as it attempts to adopt a minimum energy condition. If this condition occurs at some point around the radius edge the component will be drawn along with the droplet causing misalignment. Slight inconsistencies in the data can be observed for 5 μm and 25 μm edge radii which occur at the transition point

between the binding site top surface and curved edge models (-5 and -25 pinning position respectively). This is believed to be caused by differences in the constraints required for the different models which slightly alter the droplet shape at the transition point, resulting in inconsistencies in the resolved surface energy.

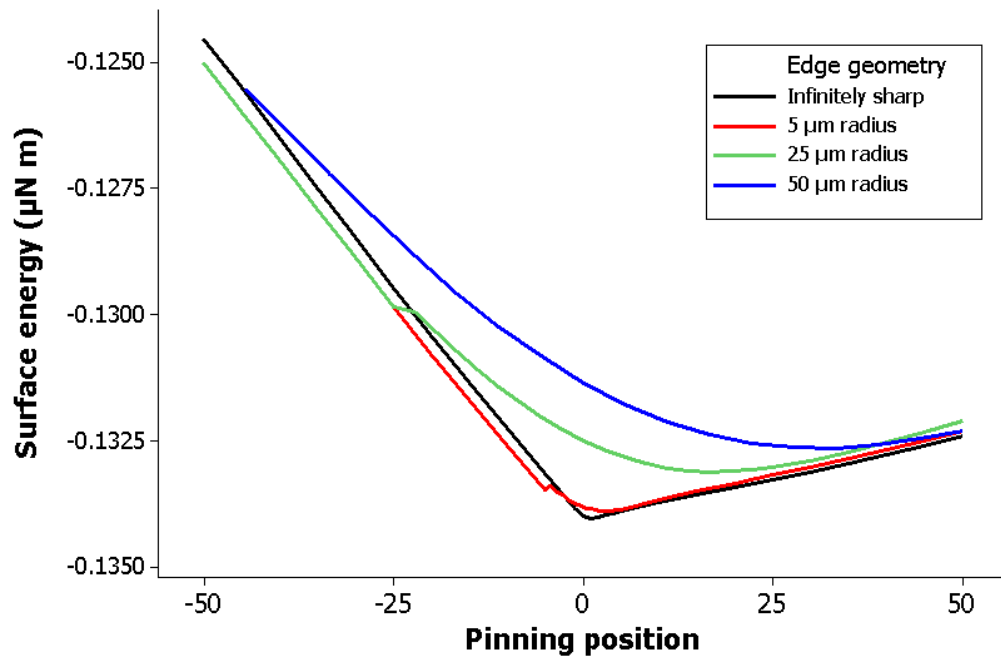


Figure 7-8: Plot of surface energy against pinning position for varying edge radius at fixed liquid volume of 360 nl.

The data show that surface energy initially starts high as the liquid droplet is in a compressed state, it then reaches a position which is the ideal state for that geometry and liquid volume and the surface energy is at a minimum. Past this point the surface energy rises again as the pinning position moves down the sidewall causing the liquid droplet to be stretched. As was shown in the models presented in the previous section, surface energy was higher for larger liquid droplet volumes. To allow a comparison of each edge geometry across the range of liquid droplet volumes investigated it was chosen to normalise the surface energy data. This does not provide a surface energy value which can be directly read from the plots, but it allows observations to be drawn from the profile of the plot and how the edge geometry behaves to changes in liquid droplet volume. The normalised data for each edge geometry was plotted

against pinning position for the range of liquid volumes in Figure 7-9. a) Infinitely sharp edge, b) 5 μm radius, c) 25 μm radius, d) 50 μm radius. Dotted lines represent the transition points between the different models.

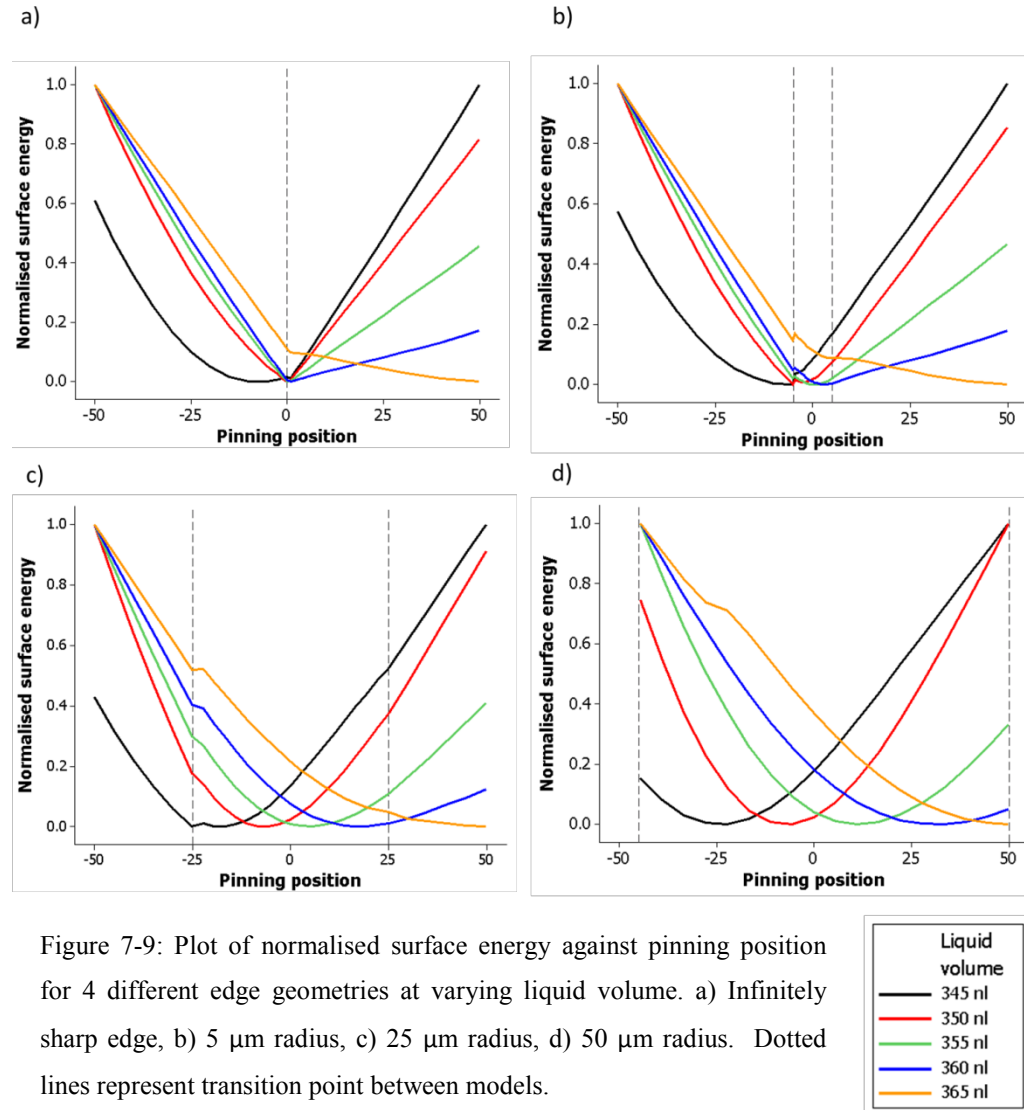


Figure 7-9: Plot of normalised surface energy against pinning position for 4 different edge geometries at varying liquid volume. a) Infinitely sharp edge, b) 5 μm radius, c) 25 μm radius, d) 50 μm radius. Dotted lines represent transition point between models.

From the data it can be seen that the behaviour of the different liquid volumes varied considerably for changing edge geometry. When the edge was infinitely sharp (i.e. no radius) (Figure 7-9 a)) the lowest surface energy state occurred at the zero position (interest between binding site top surface and sidewall) for liquid volumes of 350, 355 and 360 nl. At the smallest liquid volume of 345 nl the lowest energy state occurred on the binding site top surface. At the largest liquid volume of 365 nl the lowest energy state occurred on the binding site sidewall. It is interesting to note that at 365 nl liquid volume there was a

plateau region in the surface energy at the zero position indicating that there was an energy penalty that the liquid droplet must overcome before being able to move down the sidewall. Comparing the 50 μm radius (Figure 7-9 d)) to that of the infinitely sharp edge (Figure 7-9 a)) shows a vastly different response. Recall that in the 50 μm radius simulation all pinning positions occur around the curved edge. For 50 μm radius the point at which the lowest surface energy state occurred moved progressively further around the curved edge as the liquid droplet volume increased. The smooth shape of the plots suggests that the geometry did not offer any resistance to liquid droplet movement when the edge radius is large. The 5 μm edge radius (Figure 7-9 b)) more closely resembles the data for infinitely sharp. Although the lowest surface energy state does not occur exactly at the zero pinning position, it does occur in close proximity either side of it indicating that only small component misalignments would occur. It can also be observed that the plateau region in surface energy occurs at 365 nl liquid volume as it did for the infinitely sharp edge, albeit over a smaller range of pinning position.

The overarching observation from these series of simulations is that an increase in the radius of the edge geometry reduces the structures ability to prevent movement of the liquid droplet from the binding site top surface and down the sidewall. This is of key importance to alignment applications where the constraint of the liquid droplet to the binding site top surface is necessary to achieve accurate component alignment. Overflow of the liquid droplet from the binding site top surface as it seeks a minimum energy configuration causes the component to be drawn along with it resulting in systematic misalignment. Plateau regions were observed for the infinitely sharp and 5 μm radius edge geometries at 365 nl which suggested that these structures created an energy penalty which must be overcome for the liquid droplet to continue moving. It therefore is desirable to make the edge radius as small as possible in order to achieve this barrier to liquid droplet movement and prevent overflow of the binding site.

As mentioned earlier the model was simplified to account for only one curved edge, with the remaining edges retaining the infinitely sharp geometry. Although observations can be drawn from the behaviour of the liquid droplet for the different geometries, it is believed that some of the effects may be obscured by the inability to effectively model all four edges simultaneously. It is proposed that the surface energy would not simply exhibit a plateau region but would rather have a clear peak (Figure 7-10). This rise in surface energy would occur due to an energy penalty which must be overcome for the liquid droplet position to advance. This peak is then expected to flatten out as the edge radius increases, similar to the observations from the numerical simulations in Figure 7-9.

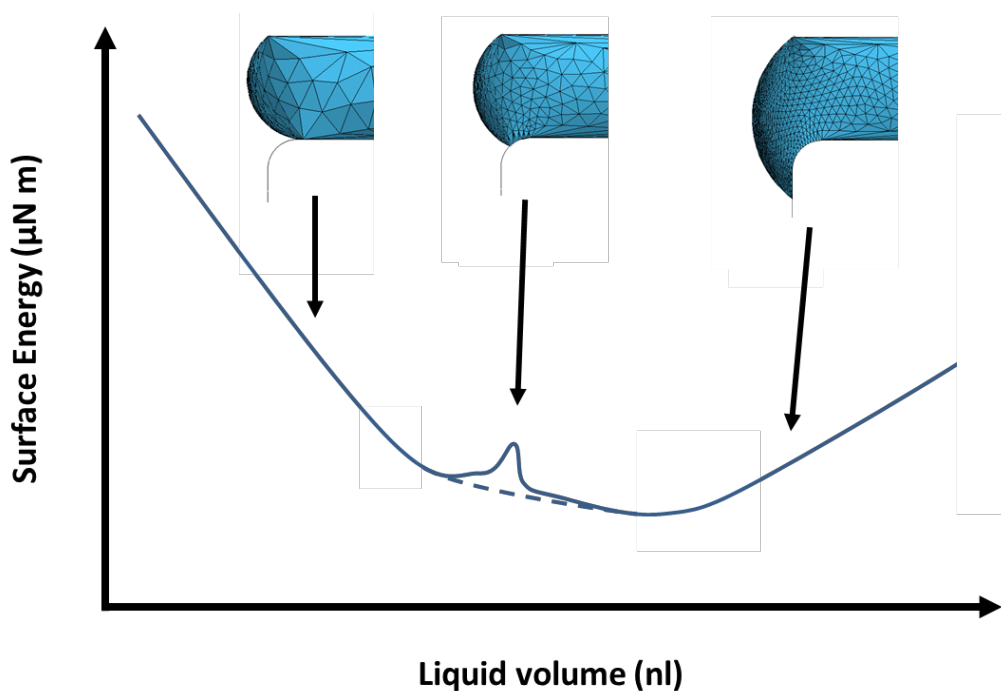


Figure 7-10: Diagram illustrating the hypothesised effect of edge radius on surface energy of a liquid droplet. Surface Evolver images show the analogous condition for each graph region investigated by moving pinning position with a fixed liquid volume. Dotted line shows hypothesised profile when binding site edge has radius.

The binding sites cross-sectioned in chapter 5, section 5.2 showed that components produced on the EnvisionTec Perfactory displayed a radius edge. Figure 7-11 shows that the extent of the radius is related to the edge geometry of the structure, with edge geometries $<90^\circ$ having a larger radius. This is

likely caused by the surface tension of the liquid resin during the curing process. From the image (Figure 7-11a)) it can be seen that for 60° nominal edge geometry (actual measured edge geometry 85°), that the radius is approximately 25 μm , whereas for 135° nominal edge geometry (actual measured edge geometry 136°) that the radius is approximately 15 μm . The experimental work in chapter 5 was unable to control the radius of the binding site edges as this is likely determined by a combination of the liquid resin surface tension and the minimum achievable layer thickness. Even though the measured edge radius of experimental structures appeared to be larger for undercuts $<90^\circ$, superior liquid containment and component alignment accuracy were observed for binding sites with undercuts $<90^\circ$. This would imply that undercutting the binding site sidewall may play a more significant role than edge radius for microdroplet alignment applications.

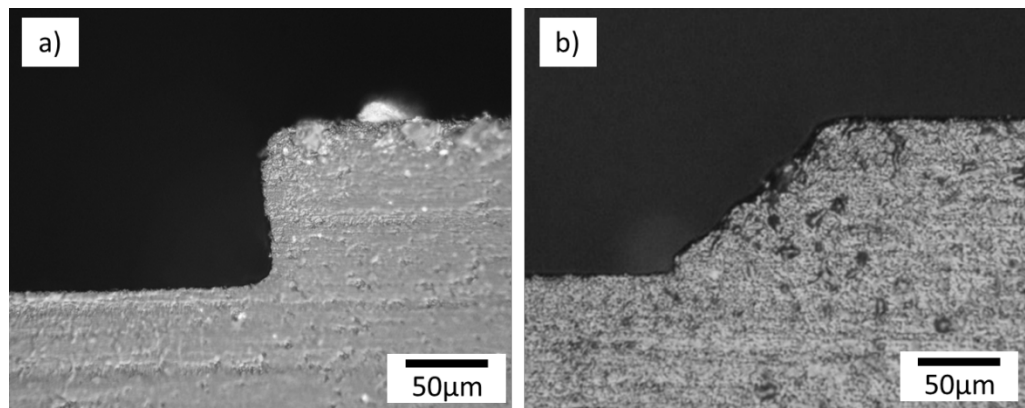


Figure 7-11: Optical microscope images of cross-sectioned binding sites. a) 60° nominal and b) 135° nominal.

7.2 Undercut structures

The containment of the liquid droplet to the binding site top surface is of key importance to successful microdroplet assembly applications. Overflow of the liquid droplet causes the component to be drawn along with the liquid which ruins the alignment process. The design of effective binding sites is therefore a key priority for microdroplet alignment to be a viable assembly technique for the micro component industry. One strategy is to undercut the binding site

structure which increases the contact angle that can be achieved by a liquid droplet according to the Gibbs inequality (chapter 2, section 2.4.12). The figure (Figure 7-12) and equation (7-2) describing the Gibbs inequality have been reproduced here for convenience.

$$\theta_c < \theta < (180^\circ - \alpha) + \theta_c \quad (7-2)$$

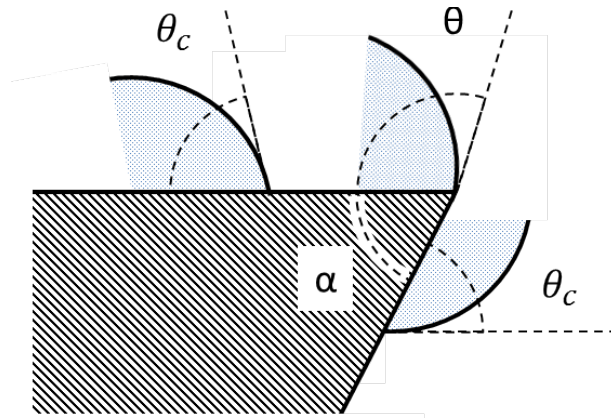


Figure 7-12: Spreading of a liquid droplet meeting a sharp edge as described by the Gibbs inequality, equation (7-2).

If the liquid droplet does overflow the binding site it is desirable to have in place a structure which discourages further motion down the sidewall which would draw the component along with the droplet and out of alignment.

Previous models presented in the literature have only considered the liquid droplet when it is pinned to the binding site top surface. The models have not taken into account the effect of the sidewall geometry and the role this plays on the surface energy of the system. The experimental work presented in chapter 5, section 5.1 suggested that the binding site edge geometry had a significant effect on the structures ability to constrain liquid droplets. It was also seen that edge geometry played a significant role in the structures capacity for alignment of micro components using liquid surface tension (chapter 5, section 5.3). Additionally it was noted that the Envision Perfactory was unable to faithfully

recreate the desired edge geometries with manufactured component undercut angles tending to be oversized.

It is therefore proposed that the surface energy penalty for a liquid droplet moving down an undercut edge $<90^\circ$ will be significantly higher than for an edge $>90^\circ$.

This section of the thesis examines the previously observed phenomena through numerical modelling using the Surface Evolver software. The model was created to represent the physical systems previously investigated in this thesis and therefore square binding sites of dimensions $2 \times 2 \times 0.1$ mm, with rectangular prism component of dimensions $2 \times 2 \times 0.5$ mm and assembly liquid of water were used (Figure 7-13).

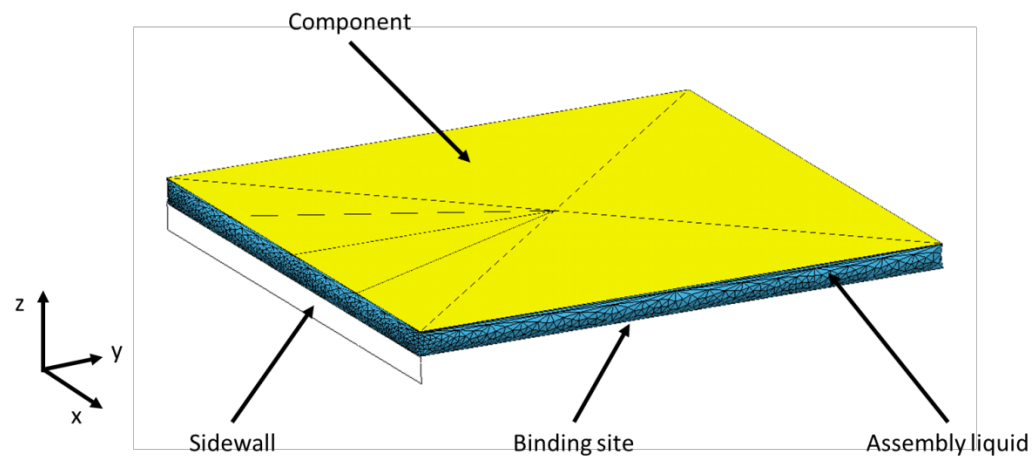


Figure 7-13: Image of Surface Evolver model created to investigate the effect of varying edge geometry.

Although the physical components manufactured on the EnvisionTec Perfactory were observed to display a radius edge (chapter 5, section 5.2), the model presented in this section displays an infinitely sharp edge so as to isolate the effect the edge geometry plays. As was introduced in the previous subsection on modelling curved edges (Figure 7-3), a challenge was unable to be resolved with the intersection of multiple constraints which caused unrealistic behaviour of the liquid droplet during evolution. The model in this

section was therefore also simplified so that only one edge featured the varying edge geometry, with the remaining three edges retaining the standard binding site geometry with the liquid droplet is pinned along the binding site top surface perimeter. The range of edge geometries investigated were undercuts of $60^\circ - 120^\circ$, in 1° increments (Figure 7-14). The model data file can be found in APPENDIX J.

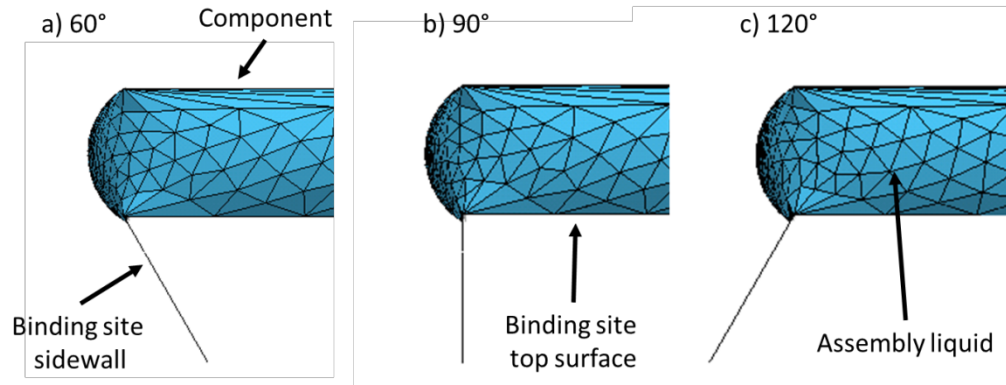


Figure 7-14: Close-up side view of Surface Evolver model showing a) 60° , b) 90° , and c) 120° edge geometries.

The droplet was pinned along the three regular edges of the perimeter of the binding site top surface, with the position of the fourth edge moved incrementally down the undercut edge in steps of 5 microns. This is illustrated in Figure 7-15 which shows the droplet edge pinned at 5 microns (left) and 50 microns (right) on a 60° undercut edge geometry.

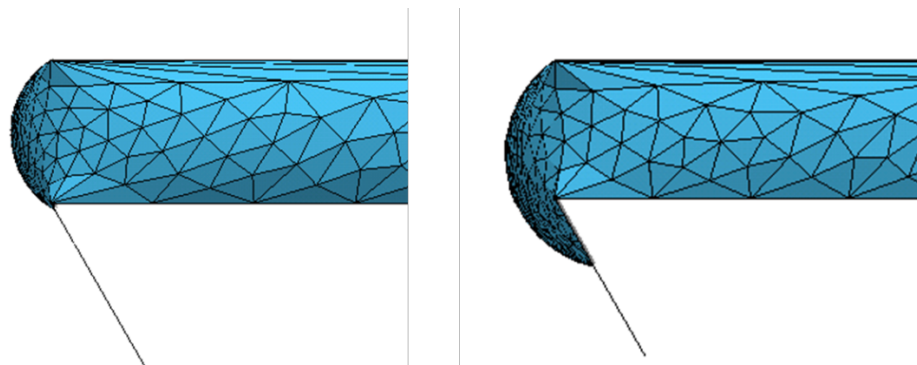


Figure 7-15: Close-up side image of surface evolver model showing different pinning position of liquid droplet on 60° undercut edge geometry for a fixed liquid volume.

The position of the component was fixed at a given distance above the binding site top surface of 87.5 μm . This was determined by dividing a liquid volume of 350 nl by the binding site cross section. The component position was chosen to ensure that the liquid droplet would be in slight compression and have sufficient volume available to wet the sidewall. The full range of edge geometries, and pinning positions were then investigated for each volume of liquid (355, 360 and 365 nl). This resulted in a total of 610 data points for each liquid volume which were then plotted as surface and contour plots to observe the effect on the surface energy of the system.

The data were presented in pairs of surface plot and contour plot for each simulated liquid volume. 355 nl (Figure 7-16 and Figure 7-17), 360 nl (Figure 7-18 and Figure 7-19) and finally 365 nl (Figure 7-20 and Figure 7-21). For these particular simulations the points of interest were the change in surface energy as the liquid droplet pinning position is incrementally moved down the sidewall from zero (intersect with binding site top surface and sidewall) to 50 μm down the sidewall. Recall that Surface Evolver aims to minimise the surface energy of a surface subject to model constraints. This means that the points of lowest surface energy identify the position that the liquid droplet will preferentially adopt.

For the lowest simulated liquid droplet volume of 355 nl (Figure 7-16 and Figure 7-17) it can be seen that the lowest surface energy occurred at the zero position across all angles of edge geometry. Highest surface energy was observed for 60° edge geometry when the liquid droplet was at 50 μm down the binding site sidewall. The surface energy was also observed to rise at a faster rate for lower angle edge geometries as the pinning position of the liquid droplet moved incrementally down the sidewall.

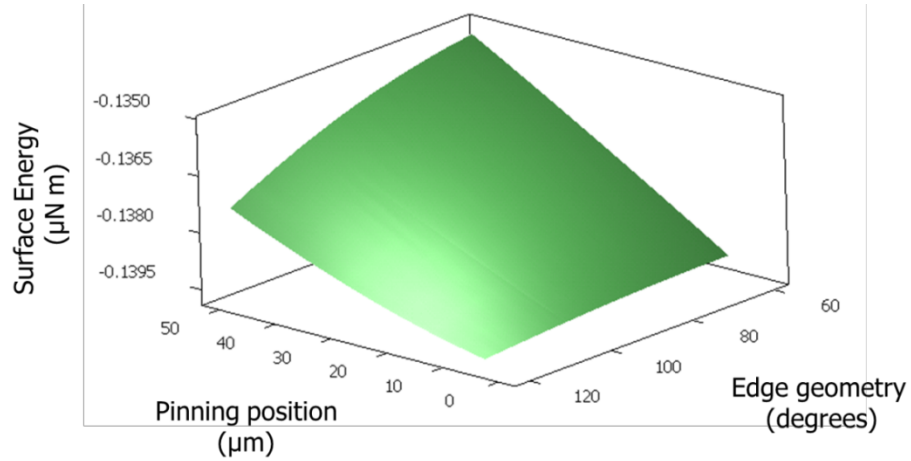


Figure 7-16: Surface plot of surface energy against droplet pinning position and binding site edge geometry for fixed liquid volume of 355 nl.

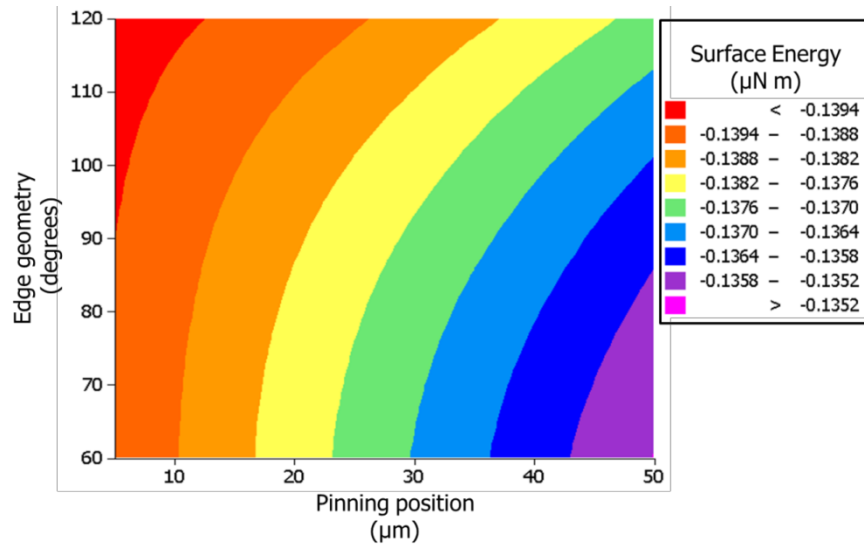


Figure 7-17: Contour plot of surface energy against droplet pinning position and binding site edge geometry for fixed liquid volume of 355 nl.

For liquid droplet volume of 360 nl (Figure 7-18 and Figure 7-19) it can be seen that the lowest surface energy position occurred at the zero position for lower angle edge geometries, however as the edge geometry became $>100^\circ$ the lowest energy state occurred further down the sidewall. At 120° edge geometry the minimum surface energy occurred at a liquid droplet pinning position of $\sim 30 \mu\text{m}$ down the binding site sidewall.

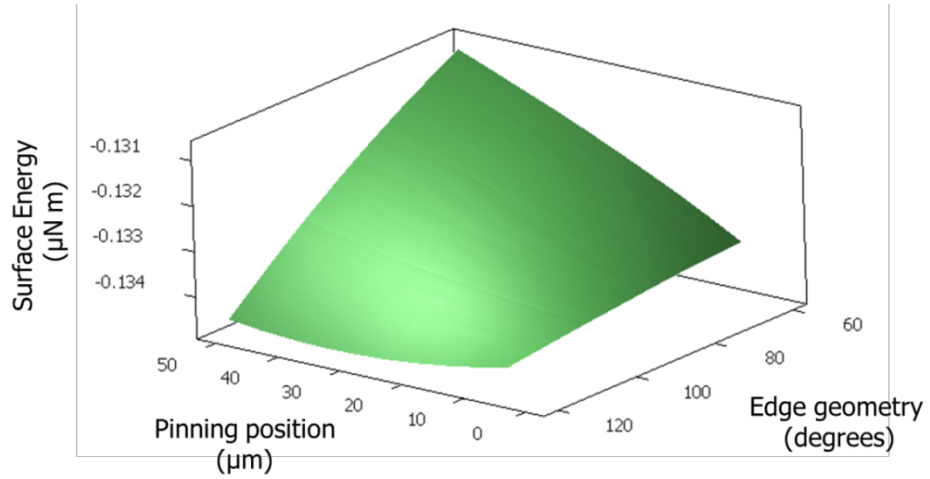


Figure 7-18: Surface plot of surface energy against droplet pinning position and binding site edge geometry for fixed liquid volume of 360 nl.

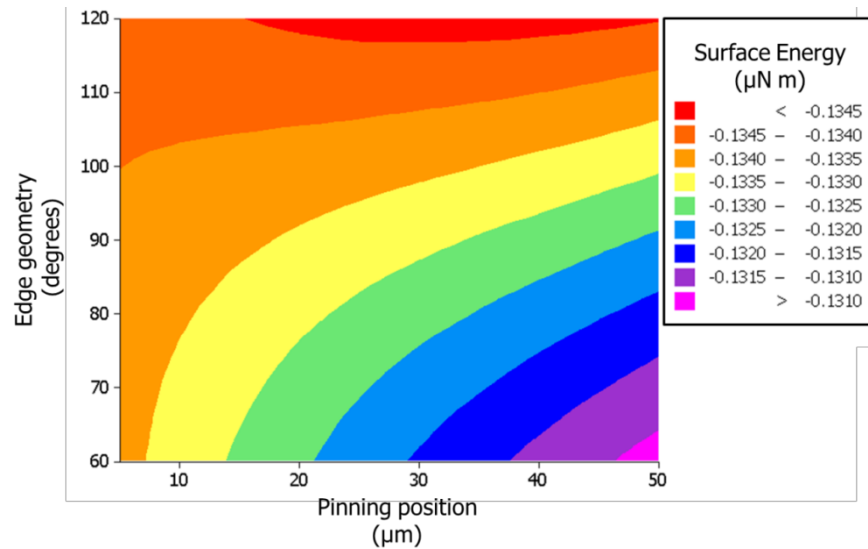


Figure 7-19: Contour plot of surface energy against droplet pinning position and binding site edge geometry for fixed liquid volume of 360 nl.

At the largest simulated liquid droplet volume of 365 nl (Figure 7-20 and Figure 7-21) it can be seen again that the lowest surface energy was obtained at the zero position for 60° binding site edge geometry, however the position of lowest surface energy changed rapidly, moving further down the binding site sidewall as the angle of edge geometry increased.

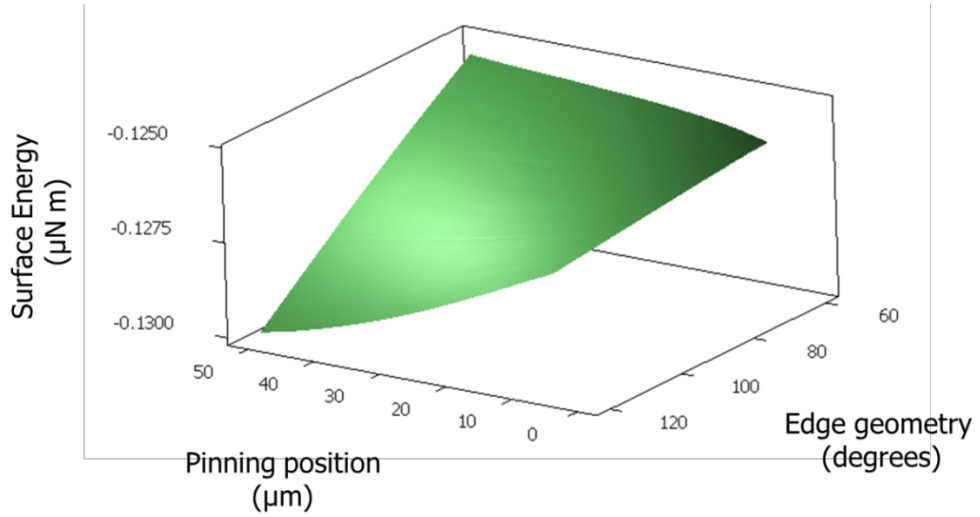


Figure 7-20: Surface plot of surface energy against droplet pinning position and binding site edge geometry for fixed liquid volume of 365 nl.

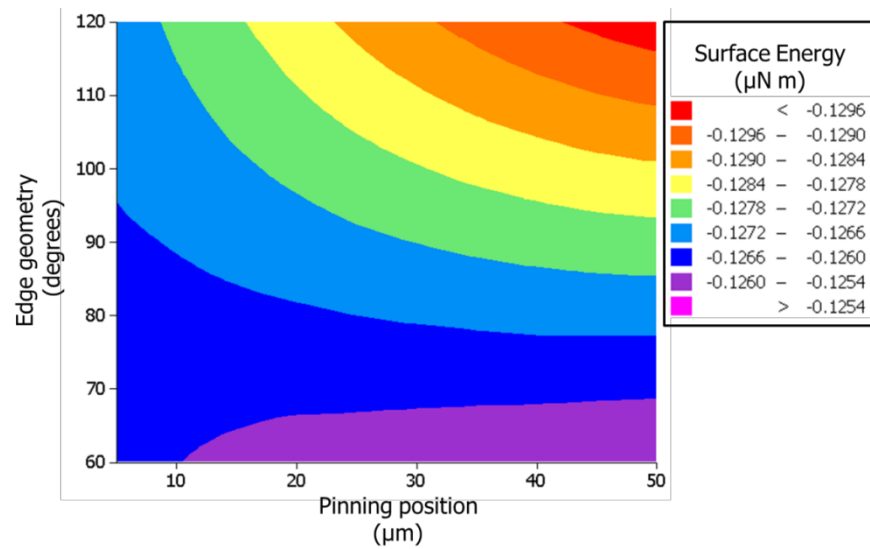


Figure 7-21: Contour plot of surface energy against droplet pinning position and binding site edge geometry for fixed liquid volume of 365 nl.

The set of simulations presented in this subsection have shown that the surface energy of the liquid droplet was highly affected by the angle of the binding site edge geometry. Undercut angles $<90^\circ$ were shown to offer a much higher resistance to droplet movement down the binding site sidewall compared to angles $>90^\circ$. In all cases 60° edge geometry (undercut) performed the best, with 120° edge geometry performing the worst. The results from the numerical simulations would indicate that it is preferential for the binding site to feature

an undercut profile in order to increase resistance to liquid droplet overflow and movement down the sidewall.

It is important to note again that the model used in this subsection was simplified to feature only one undercut edge. It is hypothesised that the trends would persist with all four edges featuring the modified geometry, and that the rate of energy change would be more pronounced between pinning positions due to the increased deformation of the liquid droplet shape with all droplet edges moving.

7.3 Summary

This chapter investigated the use of the Surface Evolver software to numerically model the effect of radius edges and undercut edges on the binding site geometry and their effect on the surface energy of the system. Interesting observations were made during the experimental work conducted in chapter 5, however limitations in the manufacturing process, such as control of the edge radius, and faithful recreation of the undercut edges, meant a detailed investigation of these factors was not achievable without a collecting a considerably larger data set which was out of the scope of this work. It was instead chosen to investigate the effects through numerical modelling where these factors could be controlled. One of the challenges that were not able to be overcome was unphysical behaviour of the liquid droplet when all four edges of the binding site were given a radius edge, or undercut. This was believed to be caused by a conflict of two intersecting constraints and a solution for this is a recommendation for future work. To overcome this limitation the models were simplified to only account for one edge of the binding site being modified.

Modelling results of curved edges showed that the surface energy of the liquid droplet is highly affected by the edge radius of the binding site. It was observed that infinitely sharp edges (no radius) produced the lowest surface energy conditions across a range of liquid droplet volumes which occurred at zero pinning position at the intersect of the binding site top surface and

sidewall. A physical liquid droplet adopts a shape in which its surface energy is minimised. The points of lowest surface energy in the numerical data therefore represent the position the droplet will preferentially adopt. If this position occurs around the curved radius or sidewall the component will not align with the binding site sidewall and will instead be drawn along with the liquid droplet resulting in misalignment of the component. It was seen that as the radius of the edge increased the binding site ability to control the motion of the liquid droplet worsened. This is in agreement with experimental data from chapter 5 where poor alignment was observed if the binding site displayed a strong radius. Plateau regions in the surface energy were observed for infinitely sharp and 5 μm radius edges at 365 nl liquid volumes around the zero pinning position which indicated the binding site geometry was creating an energy penalty which needed to be overcome for liquid droplet motion to continue. It is therefore desirable for the binding site to have the smallest achievable edge radius in order to offer the best barrier to liquid droplet movement and prevent overflow of the binding site during microdroplet assembly operations.

Surface Evolver software was used to numerically investigate undercut binding site geometries and the effect these play on the surface energy of the system. Surface and contour plots of the data were used to identify the regions of lowest surface energy for liquid droplets at different pinning positions on the binding site sidewall. Binding site structures with 60° undercut edge geometry were shown to offer the best resistance to droplet motion, with lowest surface energy states occurring at the intersect of binding site top surface and sidewall. Rapid rises in surface energy were observed if the droplet position was moved down the sidewall indicating a high energy penalty that needed to be overcome for the droplet to move. Conversely, 120° binding site edge geometry displayed the opposite behaviour, with lowest surface energy states occurring down the droplet sidewall. A rapid drop in surface energy was observed when moving down the sidewall indicating an energy benefit which would encourage the liquid droplet to move further down the sidewall. It is therefore beneficial to use binding site geometries $<90^\circ$ in order to create an energy penalty to resist liquid droplet motion down the sidewall.

Experimental results from chapter 5 showed that structures with undercut edges $>90^\circ$ achieved lower static contact angles when used to constrain liquid droplets, compared to geometries $<90^\circ$. The experimental work also showed that structures with undercut edges $<90^\circ$ offered a greater capacity for micro component alignment than structures with edges $>90^\circ$. Cross section analysis of the structures however showed that structures with edges $<90^\circ$ tended to have larger edge radii than structures $>90^\circ$ which indicated that the undercut binding site structures may play a more significant role than the edge radius, though clearly there is a strong interplay caused by the limitations of the manufacturing process.

The work presented in this chapter has shown that both edge radius and undercut angle play a significant role in the binding sites ability to control liquid droplet behaviour, which is a direct factor in the quality of alignment applications. Limitations in the presented models which consider only a single edge mean that future work will be necessary to fully understand the effects on binding site behaviour and performance.

Chapter 8

8 INVESTIGATION OF A MICRO COMPONENT TEST CASE

As was shown in chapters 6 and 7 of the thesis, Surface Evolver is a powerful tool for investigating the behaviour of surfaces shaped by liquid surface tension. However, Surface Evolver is complicated software, which requires a high level of user expertise. Training material is limited and there is a steep learning curve for new potential users. In addition there are a number of limitations to the software which prevent it being used to model complex liquid-solid interactions, so it is highly unlikely to be used outside of a purely academic research environment. To address the usability of Surface Evolver, this chapter investigates novel use strategies for the software by exploiting the dynamic modelling capability of modern Computer Aided Design (CAD) software.

CAD software is widely used in industry for the creation, modification, analysis, and optimisation of a design. Many of the commercially available packages have integrated CAE (Computer Aided Engineering) modules which allow multi-body dynamics, static and kinematic analysis of designed components and assemblies. These have a well-established user base as well as extensive company and community support. Conversely Surface Evolver has a very small user base, and no support exists outside of the user manual and tutorials.

The CAE modules mentioned above do not offer the ability to investigate fluid flow or surfaces shaped by surface tension; however they can be used to simulate the interaction of components subject to user-defined forces or spring constants. This would allow liquid-surface interaction forces generated in Surface Evolver, to be incorporated into the well understood CAE environment to optimise the design of micro components intended for microdroplet self-assembly applications.

The chapter is divided into six subsections: The first defines the problem, the second presents the general modelling solution, the third details the case study

and analytical solution, the fourth presents the creation of the Surface Evolver model along with the results, the fifth demonstrates the integration of the data into a commercially available CAE package, and finally the sixth presents an experimental investigation of the problem.

8.1 General solution

PTC Creo Mechanism was used to create a general solution to the alignment problem. The model consisted of a binding site, and component of matching dimensions, as has been presented in preceding chapters of the thesis. As Creo Mechanism cannot represent the liquid bridge, the 6 DOF were realised through individual forces acting along each axis, and torques acting around the axes (Figure 8-1). Using the data from Surface Evolver generated in Chapter 6, the appropriate force response can be applied to each axis of the model. The force applied along the x-axis and y-axis is taken from the lateral displacement case in chapter 6, section 6.3. The force acting along the z-axis is taken from the vertical displacement case (chapter 6, section 6.4). The force acting around the z-axis is taken from the torsional displacement case (chapter 6, section 6.5). Finally, the force acting around the x-axis and y-axis is taken from the tipping displacement case (chapter 6, section 6.6).

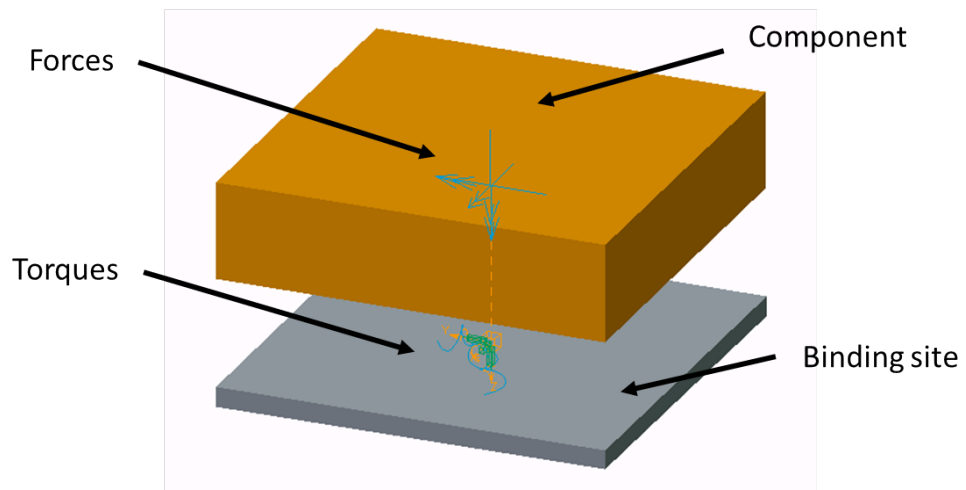


Figure 8-1: Rendered image from Creo Mechanism showing the setup of the general model.

As an example, the force acting along the x-axis of the model as it is applied in Creo Mechanism is presented in Figure 8-2. The main limitation of the general case is that it is not possible to experimentally validate the model. This would require a much more sophisticated experimental setup, capable of isolating each individual DOF.

It is important to remember that the restoring force for each DOF is only valid over small misalignments of the component. The user must therefore employ sensible initial conditions and sound judgement when drawing conclusions.

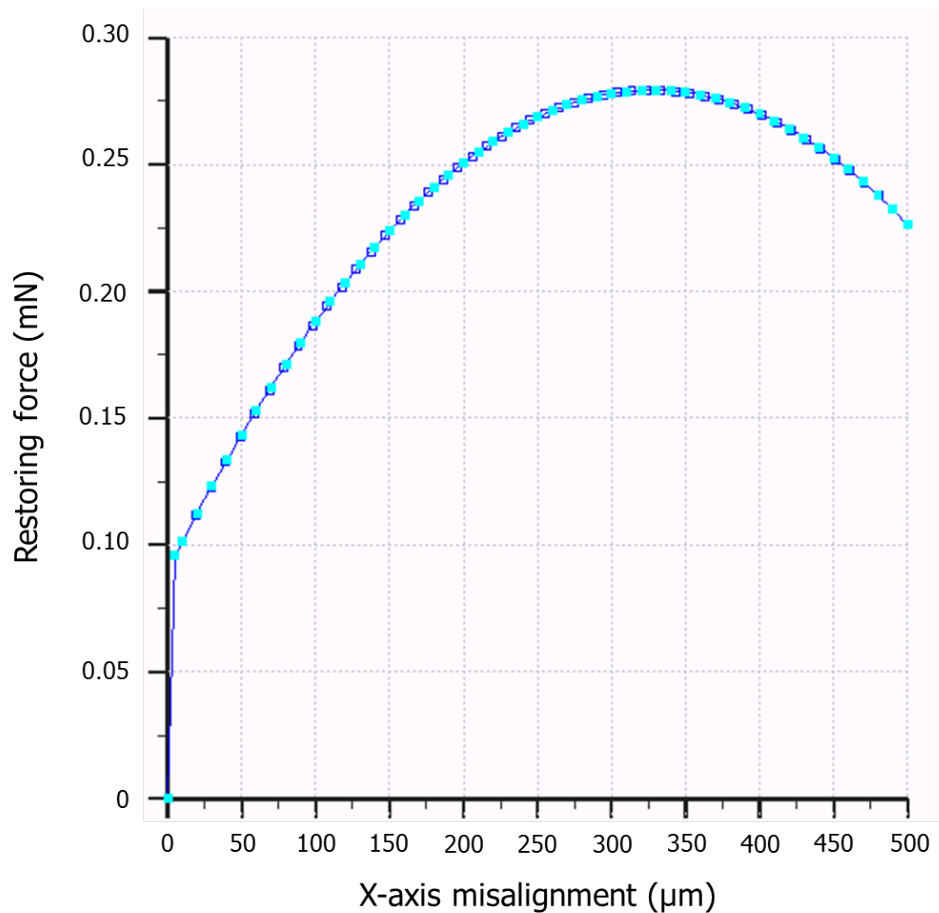


Figure 8-2: Plot of restoring force against x-axis misalignment acting in Creo Mechanism.

To demonstrate the integration of Surface Evolver data into CAD software in a practical sense, the remainder of the chapter is dedicated to that of a micro component test case.

8.2 Micro component test case

In this section the combined use of Surface Evolver with CAE software is investigated; using liquid surface tension alignment for high aspect ratio components as a case study. There are many possible case study conditions that could be explored; this chapter will present one such simple example to demonstrate how the experimental, analytical and numerical methods described above may be brought together to tackle an issue of design. The example is, that of a tall component at rest on a liquid alignment binding site which is rotated relative to the effect of gravity, observing the point at which the component would fall. The range of motion is limited to 90° , as this will produce the condition of greatest tipping moment, and is easily reproduced experimentally. As was discussed in Chapter 6, section 6.6, the restoring torque offered by the liquid droplet is very small, resulting in the component touching down onto the binding site along one edge. In this situation, lateral alignment of the component to the binding site is difficult due to frictional forces created through physical contact of the two surfaces. This case is primarily concerned with the ability of the liquid droplet to provide vertical alignment to the component, and it's alignment with the binding site below is therefore of no concern. From a design perspective this condition might also represent the mass and position of an overhanging component feature that could be supported before toppling.

This scenario is of particular interest if a designer wishes to know whether a component is suitable for microdroplet alignment and can be supported without toppling over. The integration of Surface Evolver derived forces in the CAE environment allows component design decisions and modifications to be made on-the-fly while taking into account the assembly process.

8.2.1 *Analytical solution*

Considering the geometry shown in Figure 8-3, the analytical solution for the problem was determined by calculating the moment on a high aspect ratio structure as its angle from the horizontal axis is increased. This was done by assuming that the high aspect ratio structure has a pinned joint along one edge

which acts as the point of rotation. The distance to the centre of mass of the component is then calculated as the hypotenuse of the triangle shown in Figure 8-3.

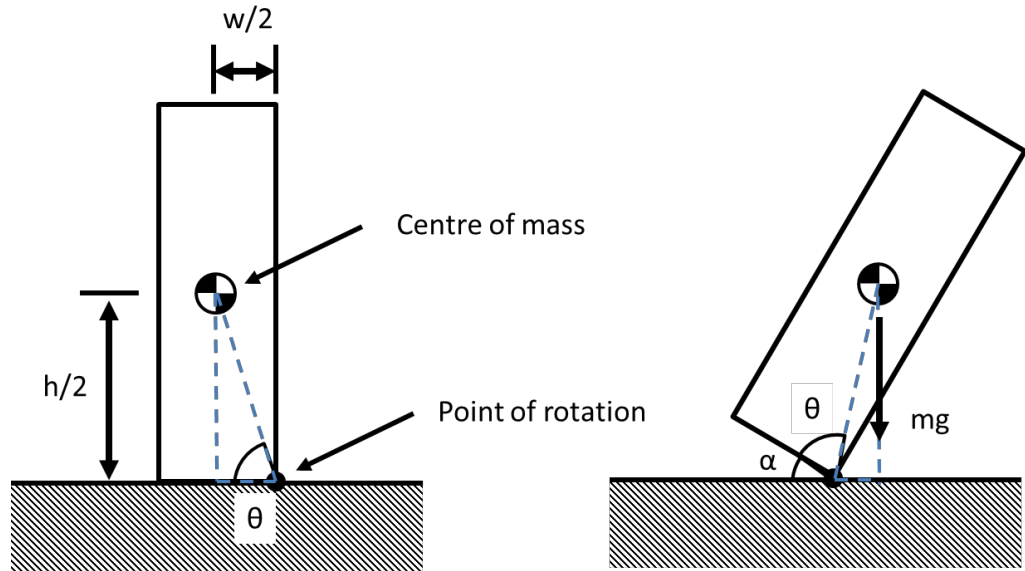


Figure 8-3: Diagram illustrating the elements of the analytical solution where h is the height of the component, w is the width of the component, m is the component mass, θ is the internal angle to the centre of mass, α is the angle of rotation, and g is acceleration due to gravity.

For each angle of rotation the length to the line-of-action of the force was calculated. This was then multiplied by the force (which consisted of the component mass multiplied by acceleration due to gravity) to determine the moment acting on the component. The experimentally derived component density was used to calculate the mass for each component (chapter 3, section 3.2.4). The results for an 8.5 mm and 12.5 mm component are plotted in Figure 8-4. It can be seen that for an 8.5 mm component the moment acts to self-right the component up to $\sim 14^\circ$ as the centre of mass is still inside the pivot point. For a 12.5 mm component this is much less, occurring at $\sim 9^\circ$. The moment generated by the 12.5 mm component is significantly higher than that of 8.5 mm and also increases at a faster rate. This is due both to the increased mass, and the increased distance to the centre of mass from the pivot point. This makes higher-aspect ratio structures much more susceptible to changes in angle. For the component to not topple over the restoring moment generated by the liquid droplet must exceed that of the toppling moment at a given angle.

In order to establish the moment generated by the liquid droplet a numerical investigation was carried out. The numerical solution for this case was modelled using Surface Evolver software and will be presented in the next subsection (8.2.2).

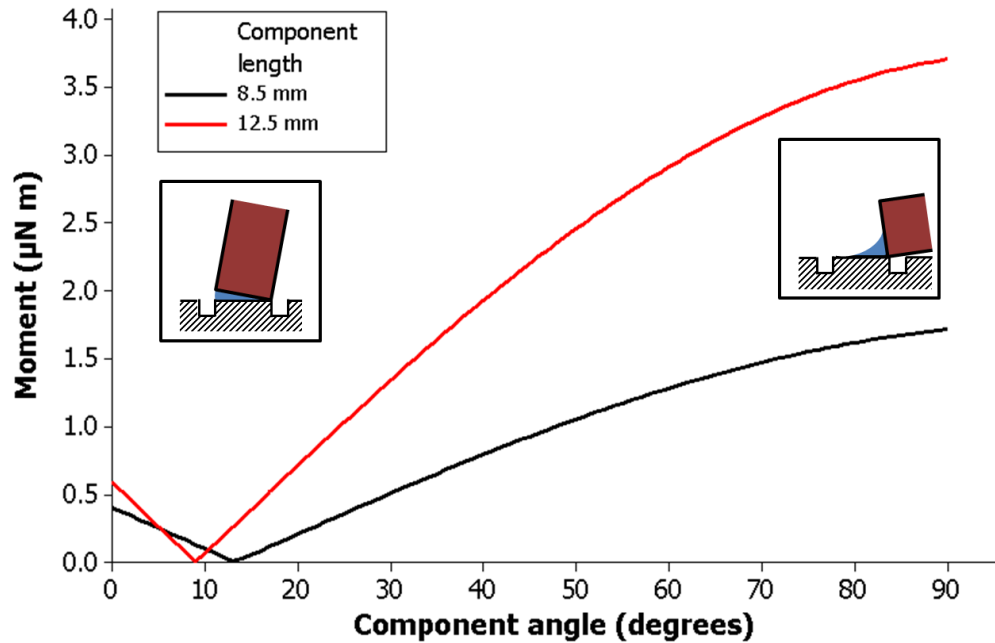


Figure 8-4: Plot of moment against component angle for analytical solution of a tipping component. Inset schematics show component (red) on binding site, supported by liquid droplet (blue).

8.2.2 Numerical solution

In chapter 6, section 6.6 the case of a component tipping about the x or y-axis was introduced. The model presented in that section was shown to not adequately simulate the case, with the component geometry passing through that of the binding site at higher angles of component rotation. When dealing with higher aspect ratio structures whose mass is considerably higher, the component finds its equilibrium position by touching down along one edge of the binding site top surface. In this subsection a new model was created using Surface Evolver to represent the effects present in the case of a high aspect ratio component whose base matches that of the binding site top surface. The model data file can be found in APPENDIX K.

If the liquid is fixed along all edges to the binding site top surface and the component, a number of issues occur as the angle between the two faces is increased. With a fixed liquid volume, an angle is reached beyond which there will not be enough liquid to fill the intersecting space between the two faces. As Surface Evolver does not account for this effect, the liquid stretches to form an infinitely thin surface. In reality the liquid would de-pin from the edge and move across the binding site and component faces, so this therefore represents an unphysical case. The phenomenon that occurs is illustrated in Figure 8-5 which shows the Surface Evolver model for a fixed volume of 200 nl. On the left, the angle between component and binding site is 2.8° , and on the right the angle is 6° . It can be seen that for the larger angle the liquid has been stretched to form an infinitely thin surface in order to obey the user-defined constraints.

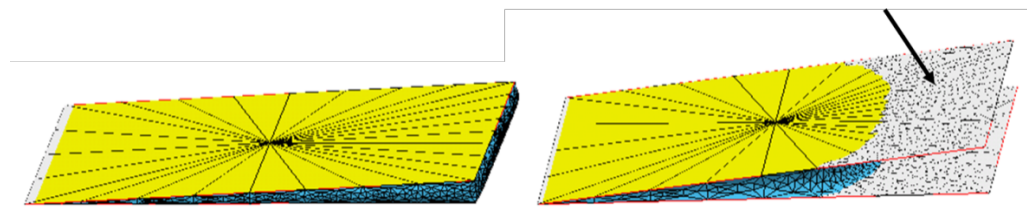


Figure 8-5: Image of Surface Evolver model showing the issue that occurs if liquid is pinned along all edges. Both images are for a fixed volume of 200 nl. (left) component angle of 2.8 degrees, (right) component angle of 6 degrees. Arrow indicates area of infinitely thin liquid surface which is an unphysical state for the system.

To overcome this, the edge of the liquid droplet furthest from the pivot point on both the component and binding site was allowed to incrementally move towards the pivot point. It was chosen to denote the pinning position of the liquid droplet as the wetted length, as illustrated in Figure 8-6.

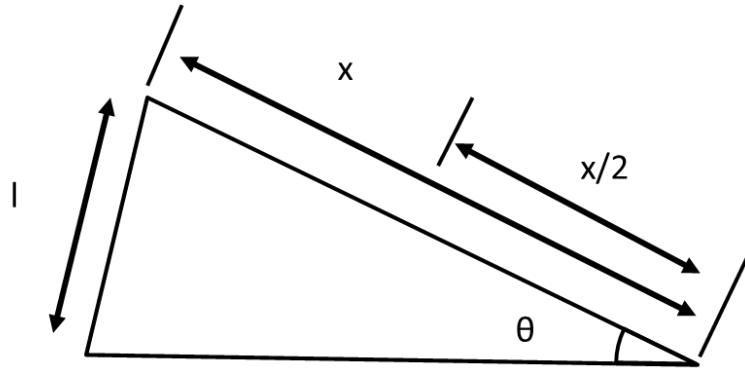


Figure 8-6: Diagram illustrating the pinning position of the liquid droplet on the binding site and component. l is chord length, x is droplet wetted length, and θ is tilt angle.

A Matlab script was written in order to batch generate the Surface Evolver data files, with the pinning position moved in increments of 0.001 cm and the angle between component and binding site increased in 0.1° degree increments. The results were plotted as a surface plot which allowed the pinning position which produced the lowest surface energy at each angle to be identified. An example surface plot for 200 nl liquid volume for the first 6 degrees of rotation is shown in Figure 8-7, and corresponding contour plot in Figure 8-8.

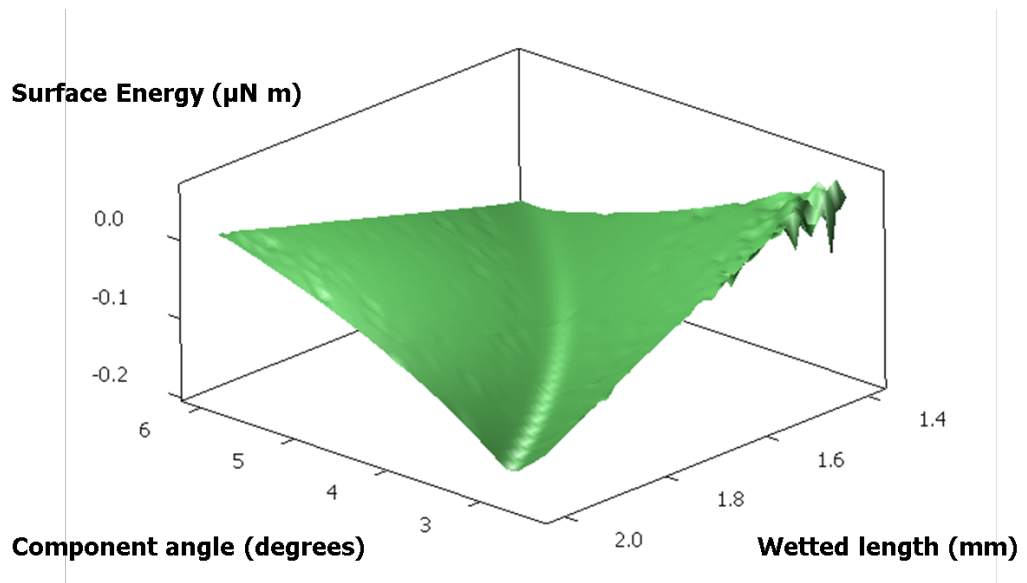


Figure 8-7: Surface plot of Surface energy against component angle and wetted length for the first 6 degrees of rotation. Fixed liquid volume of 200 nl.

It can be seen from Figure 8-7 that a trough runs through the surface plot, which is the lowest surface energy value. At a component angle of 2.5° the lowest surface energy occurs when the wetted length is 2 mm (i.e. the liquid droplet is fully wetted to the binding site and component faces). If the wetted length remains at 2 mm and the component angle increased, a rise in surface energy is observed as the liquid is pulled in tension between the faces. If the wetted length is changed to 1.5 mm and the component angle is at 2.5° the surface energy is high as the liquid between the faces is in compression, with the lowest surface energy state occurring when the component angle is at 5.2° .

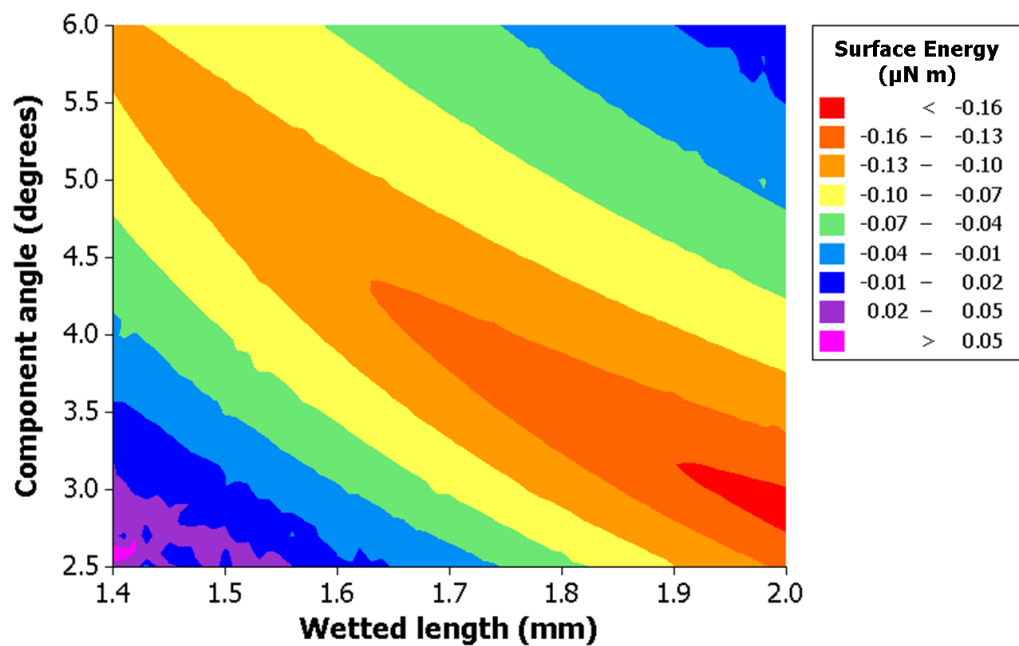


Figure 8-8: Contour plot of Surface energy against component angle and wetted length for the first 6 degrees of rotation. Fixed liquid volume of 200 nl.

Comparing the surface energy when the pinning position is allowed to incrementally move, rather than being fixed shows a significant difference as the angle between binding site and component is increased (Figure 8-9). It can be seen that when the liquid droplet is pinned along the perimeter of the binding site and component the rate at which the surface energy increases with the angle is much higher than when the pinning position is allowed to move. When differentiating this to obtain the restoring force a much higher value would be achieved therefore over predicting the amount of restoring moment

that would actually be generated by the liquid droplet. This shows that it is indeed necessary to map the whole area through the use of a surface plot to identify the lowest surface energy state for each angle of the component.

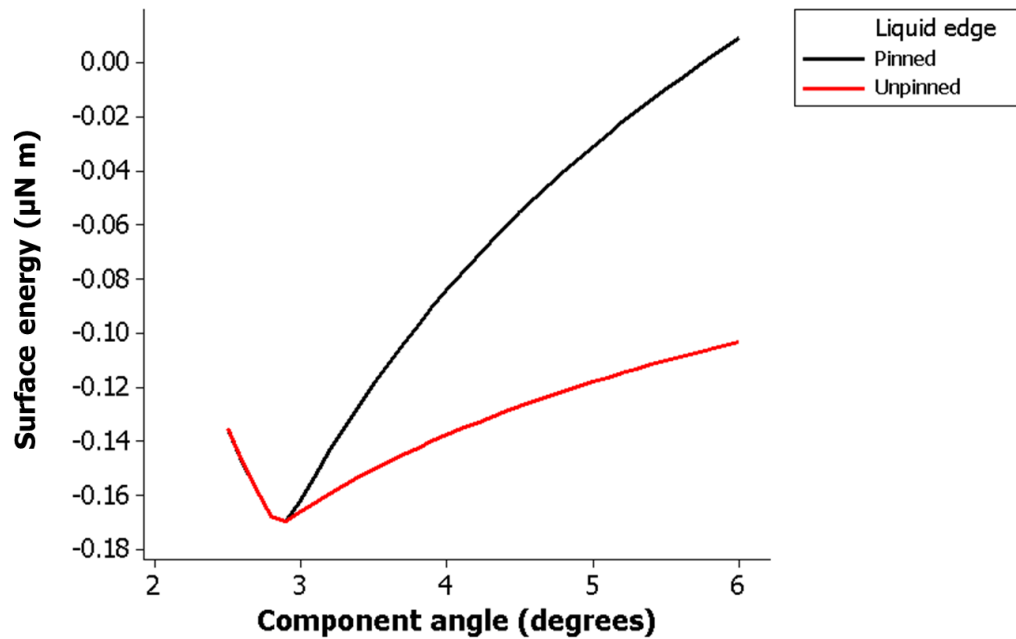


Figure 8-9: Plot of surface energy against component angle comparing the difference between pinning the liquid edge and allowing it to move. Fixed liquid volume of 200 nl.

The Surface Evolver model was used to investigate the effect of liquid volume on the tipping process. Three different liquid volumes: 200 nl, 250 nl and 300 nl were modelled and the lowest energy state for each angle of component was determined as previously described. From the graph presented in Figure 8-10 it can be seen that for each liquid volume there is an initial region of high surface energy. This is caused by the component angle being too small to accommodate the constrained liquid causing it to be compressed. Each plot has a point of inflection at its lowest surface energy which occurs at the ideal component angle for that volume of liquid. After this point the surface energy continues to increase as the component angle is increased. The rate at which the surface energy increases becomes lower as the angle increases, indicating that at higher angles the surface energy will plateau.

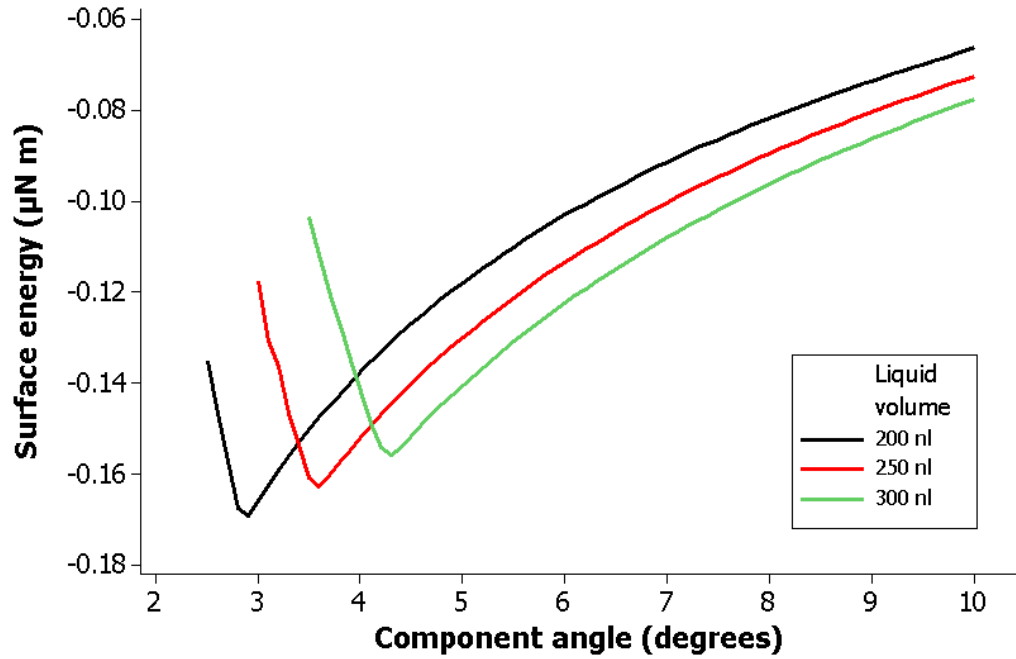


Figure 8-10: Plot of surface energy against component angle with varying liquid volume for the case of a tipping component.

The corresponding force for each component angle was calculated via numerical differentiation of the surface energy. The moment generated by the liquid droplet was assumed to act at the centre of the binding site top surface and component bottom face, with the distance from the pivot point therefore being 1 mm. The force was multiplied by this distance to obtain the restoring moment for each angle of the component (Figure 8-11). From the plot it can be seen that each liquid volume initially has a high repulsive moment acting to open the angle between component and binding site, caused by the liquid being in compression. Each liquid volume has an associated maximum restoring moment which occurs at a relatively low component angle. This then rapidly decreases as the component angle is increased and the pinning position of the droplet moves closer toward the pivot point. Highest restoring moments were observed for lower liquid volumes. From the graph it can be seen that as long as the moment exerted by the component does not exceed the maximum restoring moment generated by the liquid then the component will not topple over. Conversely if the moment of the component exceeds the initial portion of the plot acting to support the component, the liquid will be over compressed

and squeezed from between the binding site and component, thus overflowing the binding site and preventing alignment.

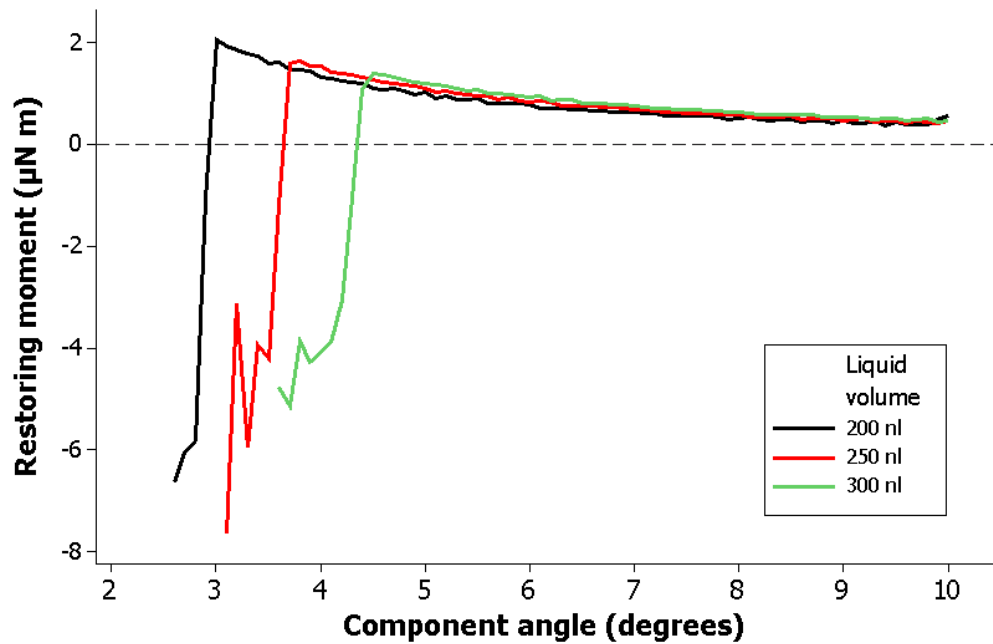


Figure 8-11: Plot of restoring moment against component angle with varying liquid volume for the case of a tipping component.

The maximum restoring moment for a given liquid volume (Surface Evolver numerical solution) and the tipping moment produced by the component (analytical solution) were compared on the same graph (Figure 8-12). From the data it can be seen that a component of dimensions 2 x 2 x 8.5 mm does not fall over across the full range of component angles from 0 - 90° for a liquid volume of 200 nl. At 300 nl liquid volume the 8.5 mm component falls over at ~65°. For the 12.5 mm component it can be seen that the component tipping moment exceeds the restoring moment of the liquid droplet for both 200 nl and 300 nl liquid volume. At 300 nl volume the maximum angle that can be achieved before toppling is ~30°, whereas for a liquid volume of 200 nl the toppling angle increases to ~42°. Although the larger component was not able to reach the same angle as the smaller 8.5 mm component, a significant level of misalignment was still achieved for a structure of 6.25:1 aspect ratio.

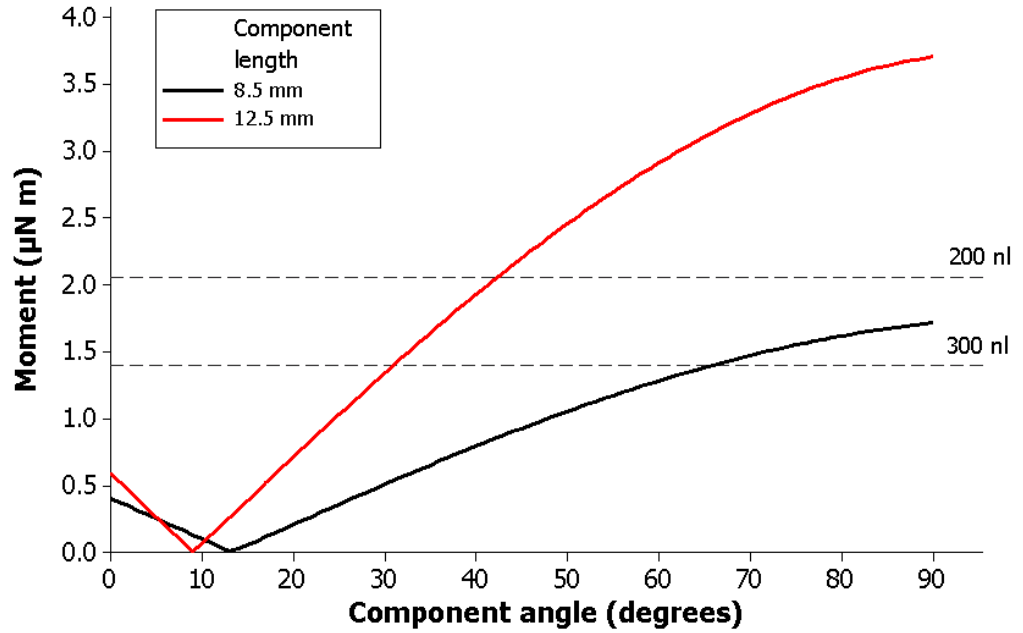


Figure 8-12: Plot of moment against component angle for analytical solution of a tipping component. Dotted reference lines show maximum restoring moment for corresponding liquid volume from Surface Evolver numerical modelling.

While the results show that liquid volume determines the amount of restoring moment that can be achieved, the size of the components heavily dominates the tipping process as their aspect ratio increases. As component size increases the rate at which the tipping moment increases will become much higher, thus cutting the two dotted restoring moment lines over a much narrower range of component angles. Highest restoring moment is seen for the lowest liquid volumes, and it is therefore beneficial to use the smallest liquid volume that is able to fully wet both the binding site and component faces to ensure a meniscus is formed. It is worth noting that as evaporation of the liquid droplet occurs; the volume will decrease, thus increasing the restoring moment generated by the liquid droplet, resulting in a larger level of component angle that can be tolerated before toppling.

8.2.3 Experimental investigation

The static and numerical solutions for the tipping of a high aspect ratio structure were previously presented in sections 8.2.1 and 8.2.2 respectively. In this subsection the two solutions were validated through a set of tipping

experiments where components of varied length in the z-axis were assembled onto matching binding sites. Binding sites were mounted on a rotating stage and a single liquid droplet applied to the binding site surface. The component was then placed on the droplet by hand using tweezers. The stage was then progressively tilted until the point of component collapse, or maximum table rotation of 66° . The full details of the experimental setup and data acquisition are detailed in chapter 3, section 3.2.10.

Square binding sites of $2 \times 2 \times 0.1$ mm surrounded by 3×3 mm trenches were manufactured using the aforementioned techniques (chapter 3, section 3.2.1), with edge geometries of 80° , 90° and 100° . Circular binding sites of equivalent surface area were manufactured resulting in dimensions of $\varnothing 2.26 \times 0.1$ mm surrounded by $\varnothing 3$ mm trenches, with edge geometries of 80° , 90° and 100° . Each binding site was manufactured twice, meaning that all structures were able to be produced on two 3×2 test arrays.

Components used in the experiments were square and circular-based prisms whose cross-section matched those of the binding site top surface. The component dimensions in the z-axis were varied from 8.5 – 12.5 mm, in 1 mm increments (5 components). The assembly task was performed 10 times for each binding site, per component. The volume of the liquid droplet was measured using the method outlined in chapter 3, section 3.2.7. The average liquid volume for experiments performed on the circular binding sites and components was found to be 255 nl with a standard deviation of 19 nl. The average liquid volume for experiments performed on the square binding sites and components was found to be 255 nl with a standard deviation of 17 nl.

The data were initially examined to establish the number of components that remained standing after the table reached its maximum rotation of 66° (Figure 8-13). From the data it can be seen that the 8.5 mm components remained standing for all three binding sites for both circular and square shapes.

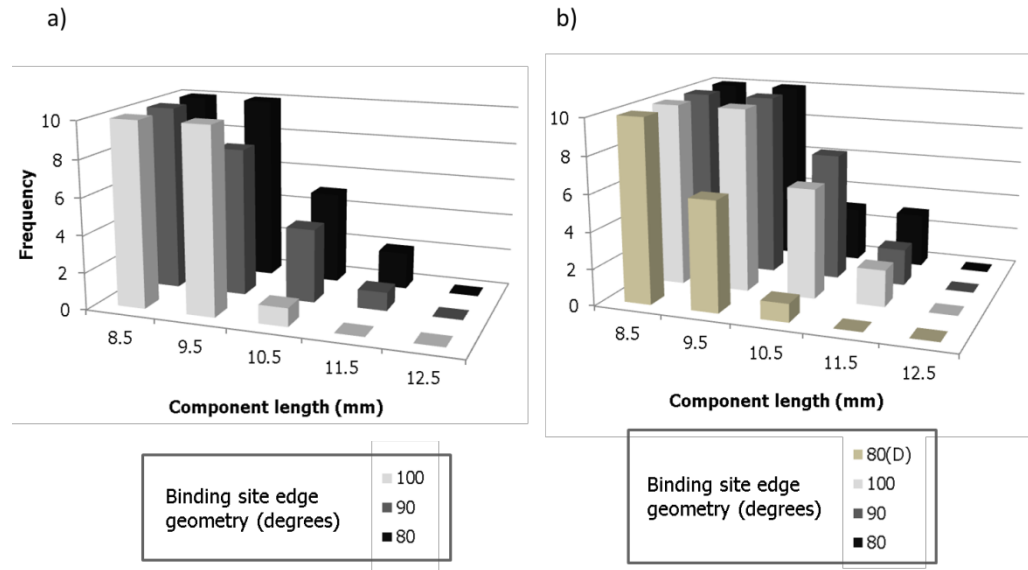


Figure 8-13: Bar charts showing the number of components that remained standing after rotating the table to maximum angle of 66°. a) Circular based components, b) square based components. 80(D) represents an 80 degree edge geometry that was found to contain a defect.

The data also show that as component length increased the number of components that remained standing at full table rotation reduced, with zero still standing at 12.5 mm length. Rather than considering the data in a binary form, furthering examination of the data for 11.5 mm and 12.5 mm length components was performed. These were chosen as >80% of the components had toppled over before reaching the maximum table angle, therefore containing data for both the angle at which the component toppled over and the measured liquid volume. This allowed a comparison between liquid volume and tipping angle to be made. The data for 11.5 mm and 12.5 mm length circular based components is presented in (Figure 8-14). The data revealed a strong negative correlation between the liquid volume and the component tipping angle. For higher liquid volumes the components tended to topple over at lower angles of table rotation. It can be seen that for 11.5 mm length components assembled onto 100° binding sites (Figure 8-14 a)) that this trend did not persist. This is thought to be caused by the large spread which can be observed in the data and may therefore be unreliable.

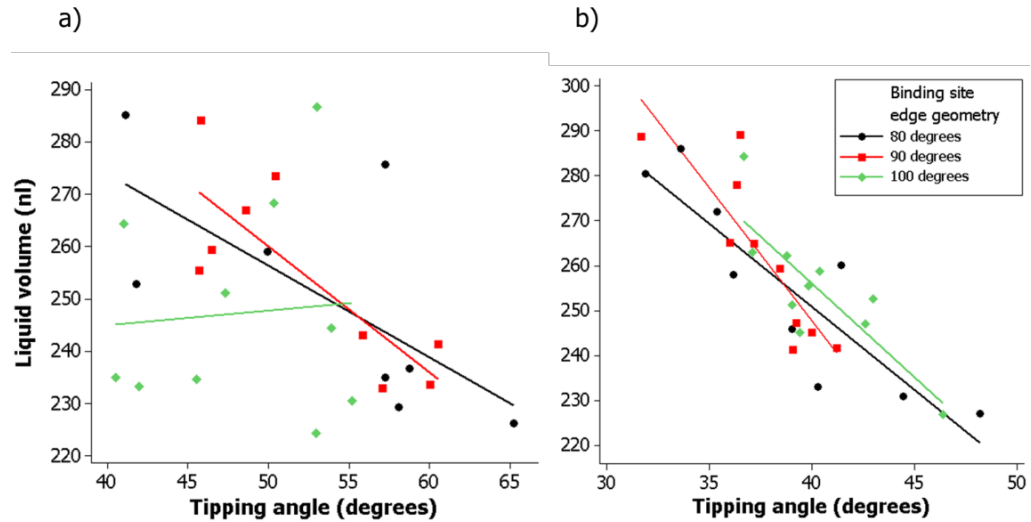


Figure 8-14: Plot of liquid volume against tipping angle of component for circular based components and binding sites on a range of binding site edge geometries. a) 11.5 mm component length, b) 12.5 mm component length. Solid lines plot a linear regression of the data set.

The data for 11.5 mm and 12.5 mm square based components and binding sites is presented in Figure 8-15. The data also showed a strong negative correlation between liquid volume and component tipping angle, which agreed with the previously presented data for circular based components.

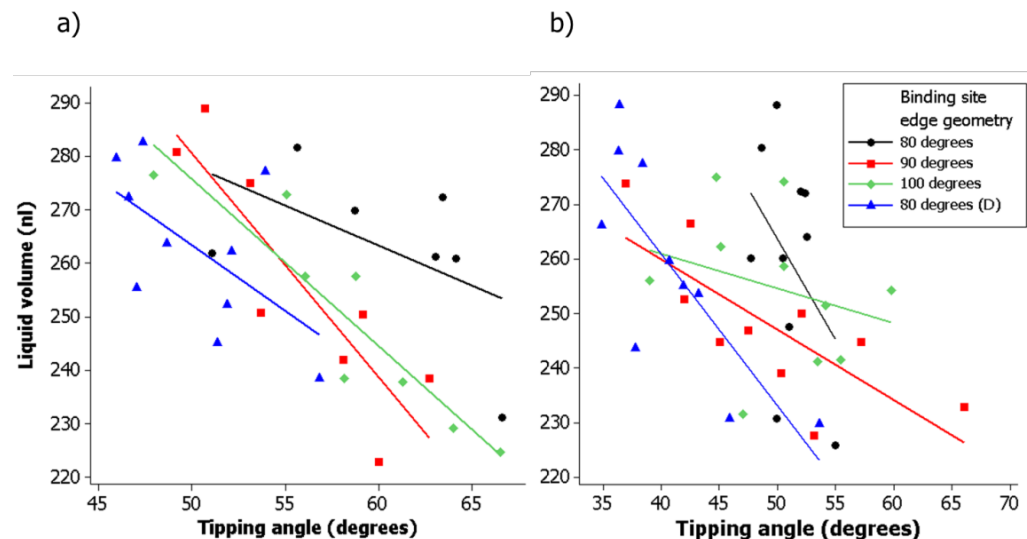


Figure 8-15: Plot of liquid volume against tipping angle of component for square based components and binding sites on a range of binding site edge geometries. a) 11.5 mm

component length, b) 12.5 mm component length. Solid lines plot a linear regression of the data set.

For the bar chart (Figure 8-13 b)) and the plots in Figure 8-15, a data series for a square binding site of 80° edge geometry was included that produced significantly poorer results compared to other binding sites. Examination of the binding site under scanning electron microscopy revealed damage to the edge of the binding site (Figure 8-16). This is believed to have allowed the assembly liquid to flow outside of the binding site causing the component to topple over at much lower angles of table rotation. This would support the observations made for the previously presented experimental work in chapter 5, and suggests that the integrity of the binding site edge is a significant factor when utilising microdroplet alignment for the assembly of high aspect ratio structures.

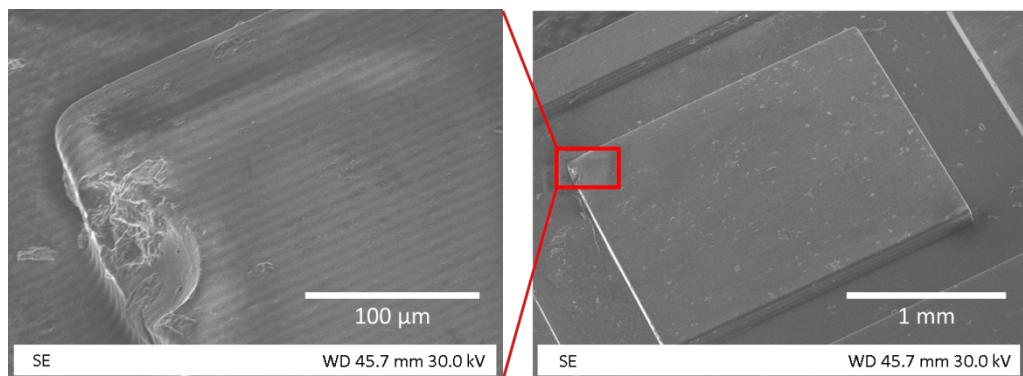


Figure 8-16: SEM image of 2 x 2 x 0.1 mm binding site with 80° edge geometry. (left) close-up of damaged edge, (right) full view of binding site.

Comparing the experimental data to that of the analytical and numerical solutions (sections 8.2.1 and 8.2.2 respectively) shows a reasonable agreement in the results. For larger liquid volumes the maximum angle a component can reach before toppling over is reduced. For the average experimental liquid volume of 255 nl, 8.5 mm length components were able to remain standing up to the maximum table angle of 66° . This is in agreement with the analytical and numerical solution presented in Figure 8-12 which showed that the moment created by an 8.5 mm component would not exceed the restoring moment generated by a liquid droplet at 250 nl.

Recall that the average experimental liquid volume was 255 nl, with a standard deviation of 19 nl and 17 nl for circular and square based component respectively. Two standard deviations from the mean incorporate 95% of the data which would give a range of $\sim 215 - 295$ nl. This falls within the range of liquid volumes (200 nl and 300 nl) examined during the numerical modelling and displayed against the analytical solution in Figure 8-12. For a square component of 12.5 mm length the numerical solution suggests that the maximum angle that can be achieved at 300 nl liquid volume before toppling was $\sim 30^\circ$, whereas for a liquid volume of 200 nl the toppling angle increased to $\sim 42^\circ$. The experimental data in Figure 8-15 b) shows that the angle at which the 12.5 mm length component toppled over was higher than the predicted values. The range of angles from the experimental data set was $35 - 66^\circ$. The discrepancy is believed to be caused due to limitations in the Surface Evolver numerical model presented in section 8.2.2. Surface Evolver is designed to model surfaces which are shaped by surface tension and other energies. Surface Evolver does not however consider solid-body interactions and therefore does not account for frictional forces, or adhesion which arises due to the contact between component and binding site which would have occurred during the experimental investigation.

8.2.4 *Integration into commercial CAE software*

The restoring moment of the liquid droplet modelled using Surface Evolver (section 8.2.2) was integrated into a commercially available CAE package. The work presented in this thesis used PTC Creo Parametric with the Creo Mechanism add-on.

The assembly model was created to represent the conditions of the analytical and numerical cases. A square binding site of dimensions of $2 \times 2 \times 0.1$ mm, and a component whose lower face matched that of the binding site surface were modelled. The component was given a pinned joint along one edge of the binding site which allowed it to rotate about one axis, relative to the binding site surface. The restoring moment was applied by connecting a force motor which acted about the pinned joint. A damper was also applied in order

to damp the oscillation and reduce the time for the assembly to settle during the analysis.

The assembly was analysed using a dynamic analysis which included the component mass, gravity, moment generated by the liquid droplet, and a damper. The damper was applied simply to reduce the oscillation of the component and reduce computation time. The force motor was defined by importing a look-up table of the moment values generated by Surface Evolver in the previous section (8.2.2). A measurement was defined to measure the angle between the binding site top surface and the component face. This allowed Creo Mechanism to identify the corresponding moment value for the force motor for a given component position within the model. For the simulations the force motor was given the data for 300 nl liquid volume generated from Surface Evolver (section 8.2.2). The system of units used within Creo was metre, Newton, second.

The initial condition for the simulation was with the component at 4° misalignment from the binding site. Recall that the range of angles generated for 300 nl in the numerical simulation was from 3.6° - 10° . In this initial condition the liquid droplet is in compression and will therefore try to open the angle until an equilibrium position is reached. The equilibrium position will therefore be a balance between the tipping moment created by the component, and the restoring moment generated by the liquid droplet. If the tipping moment exceeds the restoring moment from the liquid droplet the component will topple over.

The component designed for the simulation was a rectangular based prism of dimensions 2 x 2 x 10 mm. The component was given an overhanging feature that was 7 mm in length to create a significant moment. The dynamic simulation was run for 10 seconds and the final angle of the component then recorded. Figure 8-17 shows that the liquid droplet could not support the component in this initial configuration.

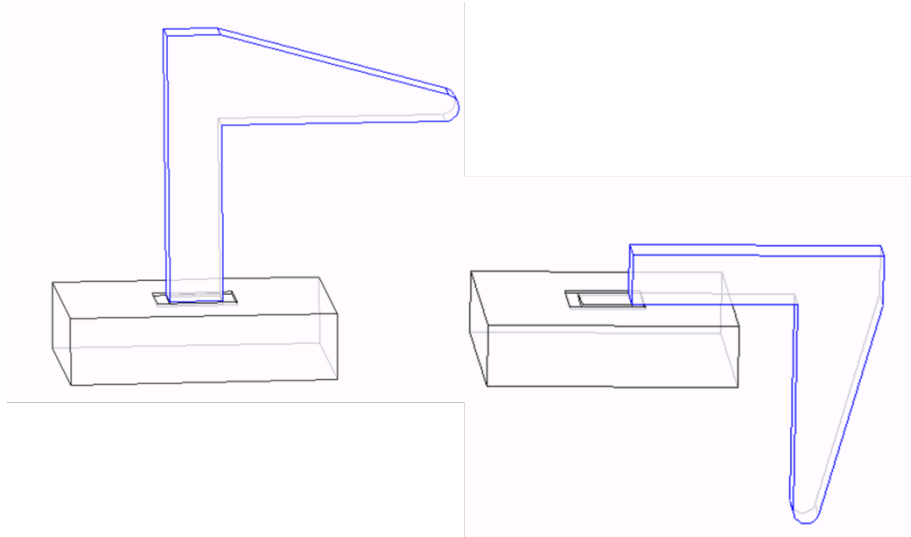


Figure 8-17: Wireframe image from PTC Creo Mechanism showing the simulated model. (left) Component at start of simulation, (right) component position at end of simulation.

The component was modified to feature a truss profile with rounded corners in order to remove mass and prevent toppling occurring (Figure 8-18). This level of geometric complexity would be extremely difficult and labour intensive to achieve within Surface Evolver, however modification and iteration of the design is extremely simple within CAD software.

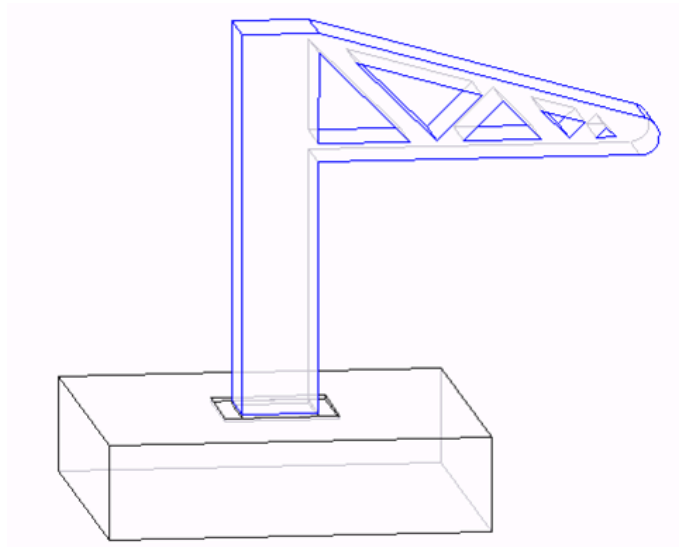


Figure 8-18: Wireframe image from PTC Creo Mechanism of modified component with truss structure.

The thickness of the truss features was incremented to find the maximum truss thickness achievable while still maintaining component alignment on the binding site. For each thickness the assembly was simulated to find the final component angle (Figure 8-19).

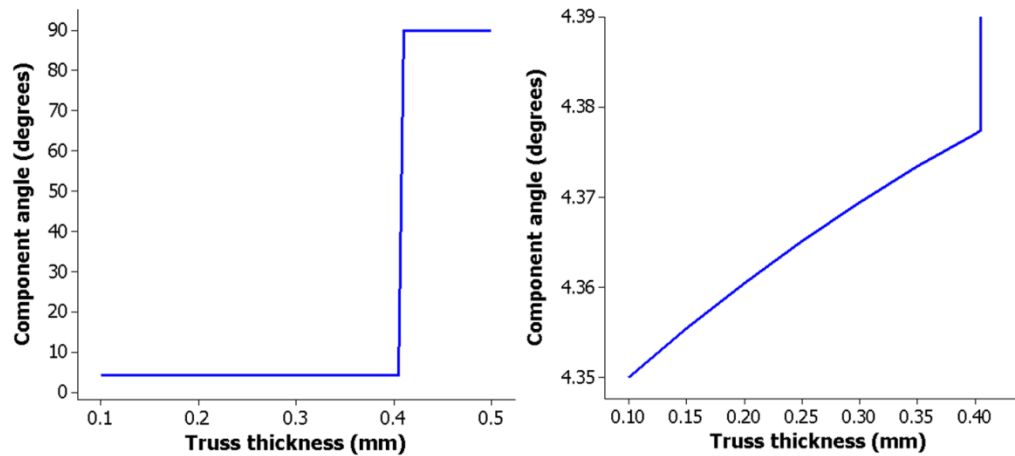


Figure 8-19: PTC Creo Mechanism simulation results showing tipping angle of component plotted against truss thickness. (left) Full range of truss thicknesses showing point of toppling, (right) Truss thickness for components that remained standing.

The data show that the maximum allowable truss thickness before component toppling was 0.4 mm. In reality a safety factor would be introduced and a thinner truss section would be selected below the maximum. Looking at the data for components that did not fall (Figure 8-19 – (right)), shows that the range of final component angles was very small which was as expected based on the small range between component equilibrium and maximum restoring moment from the Surface Evolver numerical solution in section 8.2.2 (Figure 8-11).

This work has demonstrated just one example of the application of Surface Evolver derived spring constants, integrated into a commercial CAE package for the design iteration of components intended for liquid droplet alignment. The amalgamation of these two software solutions highlights the powerful design capabilities that could be applied to micro component design and optimisation with handling and assembly techniques in mind. Once the user has established a set of spring constants for the size of binding site and liquid

droplet volume they are interested in they are able to incorporate these into a much more user friendly and flexible design package to carry out optimisation studies.

8.3 Summary

This chapter has presented the application of methodologies and models created in this thesis to create a general model as well as an example of a micro component test case. The case examined was that of a high aspect ratio structure and the resistance to toppling offered by a microdroplet when assembled on a binding site.

A new model was created using Surface Evolver to carry out a numerical simulation to address the shortcomings of the model presented in chapter 6, section 6.6. Three liquid droplet volumes of 200, 250 and 300 nl were simulated. Surface and contour plots of the resolved surface energy were used to identify the location of energy minima for each component angle as the component angle and pinning position were altered. These minimum surface energy values were then differentiated to obtain the restoring moment produced by the liquid droplet. Highest restoring moments were observed for lowest liquid volume of 200 nl. The maximum restoring moments were compared to a simple analytical solution for rectangular prism components of 2 x 2 x 8.5 mm and 2 x 2 x 12.5 mm. The data showed that 8.5 mm length components would not fall over for 200 nl liquid droplet volume, and could reach $\sim 65^\circ$ of rotation before toppling for 300 nl liquid droplet volume. At increased component length of 12.5 mm lower toppling angles of $\sim 30^\circ$ and $\sim 42^\circ$ were observed for liquid droplet volumes of 300 and 200 nl respectively. Although it has been shown that liquid volume determines the amount of restoring moment that can be achieved, the size of the components heavily dominates the tipping process as their aspect ratio increases.

A series of experiments were conducted for rectangular prism components of 2 x 2 x 8.5 mm – 2 x 2 x 12.5 mm in increments of 1 mm, and circular prism components (of comparable cross-sectional area) of $\varnothing 2.26$ x 8.5 mm - $\varnothing 2.26$ x

12.5 mm in 1 mm increments. Components were assembled onto matching binding sites with edge geometries of 80, 90 and 100°, and then tilted on a rotating stage to a maximum angle of 66°. Data showed that none of the 8.5 mm length components toppled over even at the maximum stage angle. As component length increased progressively more components toppled over with none remaining standing at 12.5 mm length when at the maximum rotation of the stage. Data displayed a strong negative correlation between liquid volume and tipping angle showing that at higher liquid volumes components tended to topple over at lower angles of stage rotation. Data were found to compare reasonably well with the numerical and analytical solutions. At the larger component lengths higher tipping angles were observed for the experimental data than the numerical and analytical solutions. This was believed to be attributed to the inability of Surface Evolver to account for the additional frictional forces caused by contact of the binding site and component. Surface Evolver is designed to model surfaces which are shaped by surface tension and other energies. Surface Evolver does not however consider solid-body interactions and therefore does not account for frictional forces, or adhesion which arises due to the contact between component and binding site which would have occurred during the experimental investigation.

As was discussed in chapter 3, section 3.2.7 the method for dispensing and measuring droplet volume results in some inherent error. Although conclusions in the experimental work presented in this chapter are drawn by comparing the liquid droplet volume against tipping angle, no specific conclusions relating to achievable angles for specific liquid volumes are made, and conclusions drawn about the trends are believed to be valid.

A design optimisation was carried out using PTC Creo Mechanism. The Surface Evolver numerical solution was applied to the model assembly in the form of a force motor. A high aspect ratio component with a large overhanging feature was designed and shown to topple over when subjected to a dynamic analysis. The component was modified to reduce the mass of the overhanging feature by applying a truss feature. The thickness of the truss was then iterated to identify the maximum allowable thickness without the

component toppling over. This complicated geometry would be extremely difficult to model and iterate in Surface Evolver.

It is believed that the integration of the two software solutions presents a novel application that addresses a complex design problem. While the test case presented here is just one example, the spring constants (once derived in Surface Evolver) can be applied to the design and optimisation of any component intended for microdroplet alignment applications.

Chapter 9

9 CONCLUSIONS AND FUTURE WORK

The work presented in this thesis was carried out with the aim to **develop an improved understanding of how liquid surface tension controls component alignment with a focus on factors associated with fabrication quality; offering insight into the impact of adopting the novel additive manufacturing route, and to provide means for designers and engineers, who are not intimately familiar with the dynamics of liquid alignment, to incorporate such features into their work.**

A critical review of the literature regarding micro components, micro assembly and handling, microfluidics, the physics of liquid droplet assembly, computational analysis for microfluidics, and manufacturing methods was performed. This review identified the three following knowledge gaps.

- **Lack of a methodology for the design of additively manufactured components for microdroplet alignment.**
- **Lack of intuitive numerical modelling tools to aid in the design of structures for microdroplet component alignment**
- **Lack of numerical model to assess the effect of non-idealised edge geometries**

These knowledge gaps were addressed by a program of experimental investigation and modelling. A suitable additive manufacturing process for the production of liquid alignment binding sites was characterised. A range of binding site geometries and configurations were manufactured using a projection microstereolithography process to establish design rules for the fabrication of functional structures.

The effect of binding site edge geometry on the ability to control liquid spreading was investigated both experimentally and by numerical simulation. A series of challenging assembly tasks were carried out to assess the manufactured binding sites' ability to offer precision alignment for components. Following these observations a series of models were created using the free-to-use software Surface Evolver to carry out numerical simulations which examined binding site edge radius, and binding site undercuts. These models expressed the forces generated by a liquid droplet under typical self-assembly conditions. Models were created using Surface Evolver and used to simulate a component while under different misalignment conditions which constituted the six degrees-of-freedom of the component.

The above models and insights were used to design components for a micro component alignment test case. The case presented was that of a high aspect ratio component. A model was created using Surface Evolver and compared to a simple analytical solution, and experimental investigation. The simulation output from Surface Evolver was integrated into PTC Creo Mechanism to demonstrate the design flexibility offered by an intuitive design tool. An optimisation study was performed on a test case for a high aspect ratio component, thereby demonstrating the feasibility of a flexible design tool for component optimisation.

Finally it was observed there was a lack of a numerical model to assess the effect of non-idealised edge geometries on binding sites used for liquid droplet alignment. A series of Surface Evolver models were created to examine the effect that binding site edge radius and undercut structures played on the liquid droplet during component alignment.

9.1 Key findings

Having reiterated the knowledge gaps and how the work in this thesis contributed to addressing them, the focus now moves to discussing the key findings of the research project.

The feasibility of utilising additively manufactured binding sites for liquid droplet alignment tasks was established. Components were manufactured on an EnvisionTec Perfactory which is a PMSL machine, using EnvisionTec R11 resin. A series of design iterations were performed to establish a set of design rules which allowed a high yield rate of binding sites and components free from significant defects to be manufactured suitable for experimental investigation. Liquid water droplets were applied to circular and square binding sites and their volume incrementally increased until the point of collapse. Binding sites were shown to constrain the movement of the triple contact line of the liquid droplet at the binding site edge leading to a significant increase in the measured static contact angle up to 158° , compared to 70° for a droplet placed on a plain flat substrate. A decrease in the contact angle was observed for binding sites where the nominal edge geometry was greater than 90° , compared to binding sites with nominal edge geometries less than 90° . Three challenging component assembly tasks were performed to establish the binding site structures' ability to offer precision alignment. Rectangular prism components were assembled onto square binding site and the difference between their centres measured to establish positional accuracy. Clear benefits were observed for structures with actual edge geometries $<90^\circ$ which achieved repeatable alignment for an alignment threshold of $25\text{ }\mu\text{m}$, with a mean final component misalignment of $31\text{ }\mu\text{m}$ and $14\text{ }\mu\text{m}$ standard deviation. Cross-sectional analysis of the structures revealed that the manufacturing process struggled to faithfully recreate the nominal angles, with actual edge geometries tending to be oversized. SEM imaging showed a distinct stepping of the individual layers for structures with actual edge geometries $>100^\circ$ which was seen to have a significant negative effect the self-alignment process if the droplet overflowed the top layer of the binding site.

A series of models were created using Surface Evolver which examined the alignment of a component subject to different states of misalignment which accounted for the 6-DOF of the component. Batch scripts were written in Matlab to allow a large number of data files to be generated for simulation. The integration of Surface Evolver generated spring constants into a

commercial CAE package for the purpose of an optimisation design study was presented. The optimisation of a high aspect ratio component was demonstrated which highlighted the potential of the technique for analysing complex geometries which would otherwise be extremely difficult if carried out purely in Surface Evolver.

Surface Evolver was used to examine the effect of imperfect binding site edge geometry on the behaviour of liquid droplets during the alignment process. To the authors knowledge this is the first presentation of a liquid droplet confinement model that can account for edge imperfections. Two edge geometry considerations were modelled; edge radius and undercut angle. Simulations of edge radius showed that for an infinitely sharp edge (no radius), the lowest energy state occurred at the intersection between binding site top surface and sidewall. As the edge radius increased, the lowest surface energy position of a liquid droplet moved further away from the binding site top surface and around the curved edge. Liquid droplets aim to minimise their energy, so this lowest energy state represents the position the droplet will preferentially adopt. This has implications on the binding sites ability to offer accurate component alignment as component position is determined by the behaviour of the droplet. If the position with the lowest energy state for the liquid is when the droplet is around the curved edge or on the sidewall this will cause component misalignment. Simulation of undercut angle showed that binding site geometries $<90^\circ$ created a high energy penalty for a droplet moving down the sidewall. In contrast, binding site geometries $>90^\circ$ created an energy benefit with lowest surface energy positions occurring down the sidewall. This is in agreement with the experimental data from previous work in the thesis which showed lower liquid droplet contact angles were observed when binding site undercuts were greater than 90° , compared to geometries $<90^\circ$. It is important to consider that both models were simplified to only simulate the effect of imperfect geometry on one edge. This was due to an unresolved challenge caused by a conflict in the constraints function of the surface evolver software, the solution to which is suggested as an area for future work.

A novel use of a nanoindenter machine was demonstrated by probing a liquid droplet and measuring the response. A replacement indenter tip was additively manufactured similar to the binding site and components which had previously been experimentally examined. Observations were drawn from the data which displayed clear events which were described according to the author's observations from previous experimental behaviour. Liquid droplets were found to achieve a maximum force of $\sim 3 - 5$ mN before overflowing the binding site which were comparable to numerical results obtained in Surface Evolver. This work has demonstrated the feasibility of a nanoindenter machine to be used to carry out novel measurements of liquid droplet mechanics and dynamics. A similar technique could be applied to other applications, for example tensile tests on micro components, using an AM rig compatible with the nanoindenter.

9.2 Recommendations for future work

The research work presented in this thesis has achieved the project aim by addressing the proposed objectives, and in addition has identified new opportunities for future work which would build on the findings presented.

The modelling of non-ideal binding site edge geometries using Surface Evolver revealed that edge radius and binding site undercut played a significant role in liquid droplet behaviour, and therefore alignment quality. The models presented in the thesis were simplified to examine only a single edge due to an unresolved challenge which caused modelling errors when applied to all edges. Future work could focus on addressing this modelling challenge. This could be achieved by resolving the conflict between constraints which was believed to be the cause of the errors encountered. Alternatively the energy change caused by the edge geometry could instead be accounted for through the use of the energy integral function within Surface Evolver which would remove the need for constraints to define the edge geometry.

Binding sites examined in this work were limited to simple geometries of squares and circles. Future work could focus on the use of complex binding

site geometries with a view to achieve specific tasks. These could be investigated for applications other than assembly, for example being used to provide rotational resistance to a component. The work in this thesis also focused on the use of only a single binding site. Future work could examine the behaviour of multiple binding sites, potentially of different geometries, to provide more flexible assembly solutions.

The integration of Surface Evolver derived data into a commercial CAE package was demonstrated for an example micro component test case. To create a truly flexible design tool a database of spring constants would need to be established which accounted for size and shape of binding site, as well as liquid droplet volume.

The method used in this thesis for dispensing liquid droplets meant that accurate and repeatable control of liquid droplet volume was not possible. Droplet volume was measured for each experiment by measuring its profile from a top-down image followed by numerical calculation. Dispensing systems offering very precise control of liquid volume are available, however these are very expensive and highly inflexible. The development of a new liquid droplet dispensing is therefore recommended for future work.

The recommendations for future work mentioned above would all contribute to an increased understanding of liquid droplet alignment. The ultimate aim would be to create a fully-fledged suite of tools which could be included in commercial CAD/CAE software to allow intuitive design decisions to be made by the designer or engineer when optimising products for micro droplet alignment tasks.

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Appendices

APPENDIX A - Self-assembly of components using liquid surface tension

The following appendix presents the experimental data in its entirety for *case b*) twist offset (Figure A-1), and *case c*) droplet misalignment (Figure A-2).

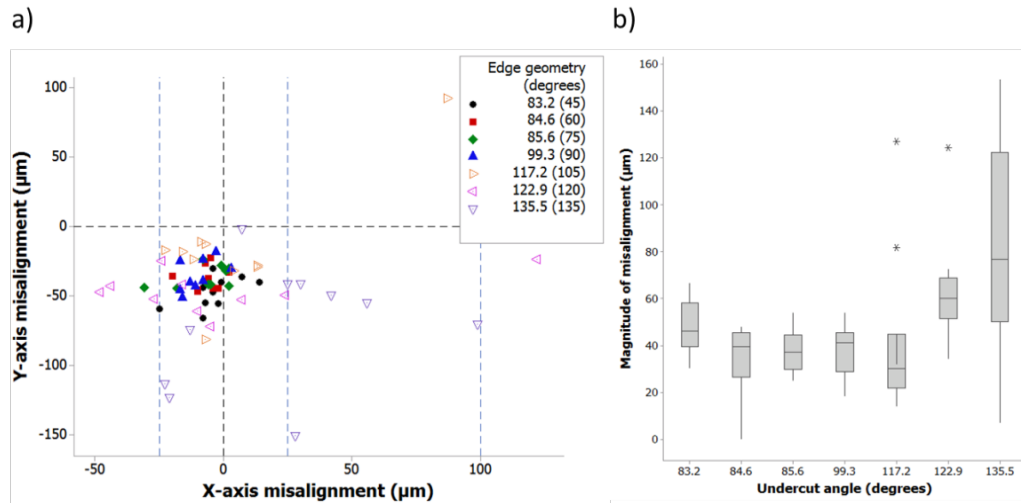


Figure A-1: Assembly results for twist offset tests: a) scatter plot and b) box plot. Dotted lines indicate threshold regions of 25 and 100 μm misalignment in the x-axis. Numbers in brackets represent the nominal edge geometries. Asterisks indicate outliers in the data.

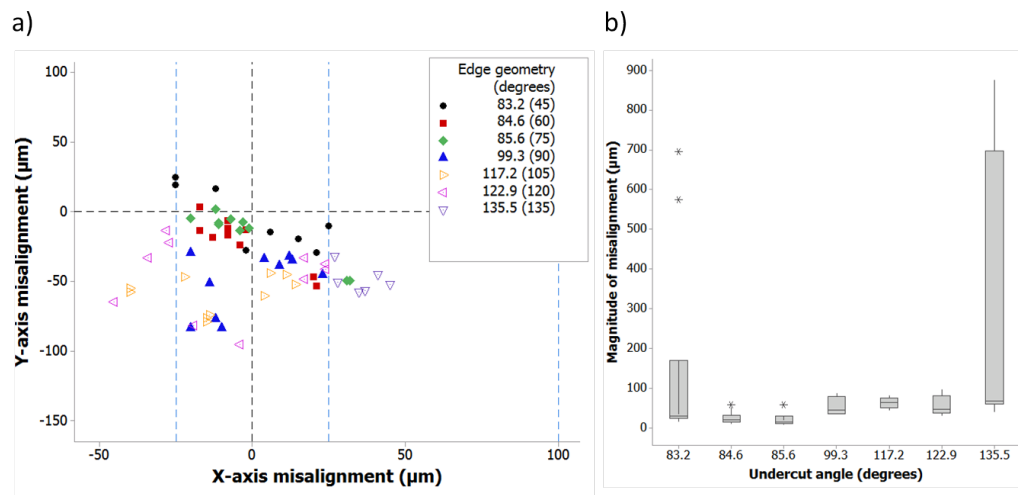


Figure A-2: Assembly results for droplet misalignment tests: a) scatter plot and b) box plot. Dotted lines indicate threshold regions of 25 and 100 μm misalignment in the x-axis. Numbers in brackets represent the nominal edge geometries. Asterisks indicate outliers in the data.

APPENDIX B - Background readings for nanoindenter

Background readings were collected to establish the behaviour of the Agilent G200 nanoindenter. The data were split into loading and unloading and then fitted with a 5th order polynomial. These were then used to remove the background data from the experimental data sets.

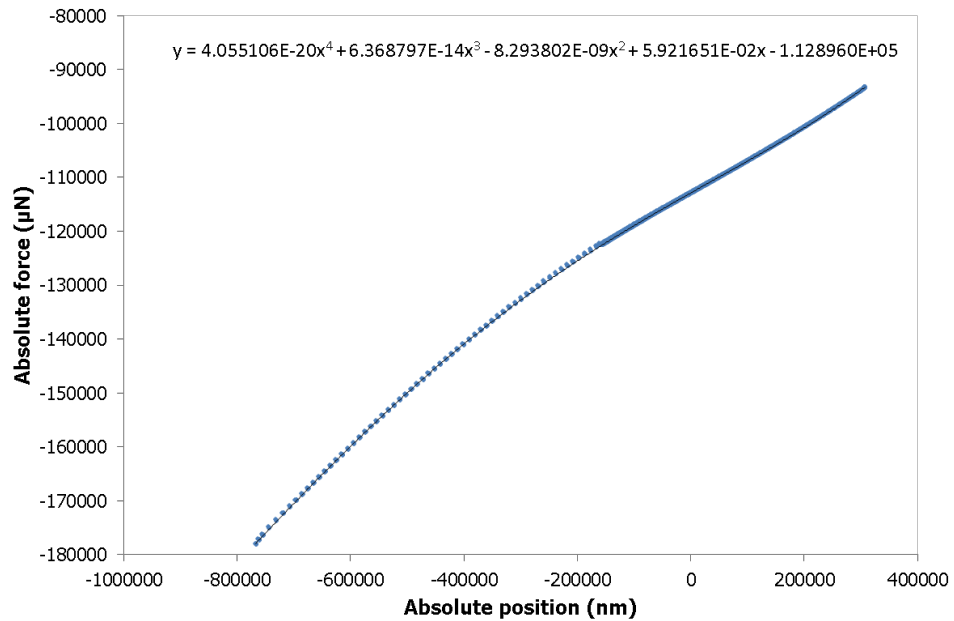


Figure B-1: Loading portion of the background reading obtained from Agilent G200.

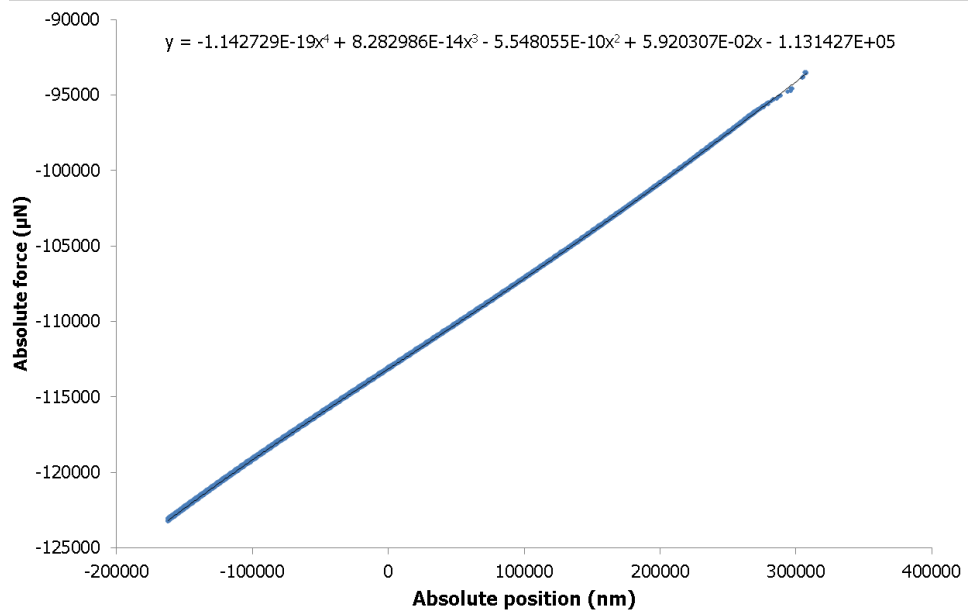


Figure B-2: Unloading portion of the background reading obtained from Agilent G200.

APPENDIX C - Introduction to Surface Evolver

The following appendix is intended to introduce the reader to the Surface Evolver software and is divided into two sections: The first is provided to familiarise the reader with the terminology and operation of the software. The second section highlights areas of the software that are of key importance to designing successful models and the authors own recommendations.

C.1 Introduction to Surface Evolver

Surface Evolver is a free-to-use software package developed by K. Brakke at Susquehanna University, PA. It is an interactive program for studying surfaces that are shaped by surface tension and other energies. Surface Evolver simulations are subject to a number of user defined energies including surface tension, gravitational energy, squared mean curvature, user-defined surface integrals, or knot energies. It is also able to incorporate volume constraints, boundary constraints, and boundary contact angles.

Surface Evolver is non-dimensional and the user must therefore comply to a consistent system of units, for example centimetre, gram, second (CGS), or meter, kilogram, second (MKS). Each evolution of the model is referred to as an iteration. Surface Evolver calculates each iteration by first calculating the force on each vertex from the gradient of the total energy of the surface relative to the vertices position. This force gives the direction of motion for the vertex which must conform to any applicable constraints. Finally the actual motion is then determined by multiplying the force by a global scale factor. The output from the Surface Evolver models is surface energy:

$$E = \gamma S \quad (C-1)$$

where E is the surface energy, γ is surface tension, and S is the interfacial area of the liquid.

When simulating the evolution of liquid droplets the interfacial area is determined by the droplet surface area that borders any wetted surfaces and surface area that is not wetted, i.e. that which is in contact with air.

Unlike commercially available simulation software packages such as ABAQUS [183], COMSOL Multiphysics [184], or CAD, Surface Evolver does not contain a graphical user interface, or drawing tools for the construction of the models. Instead models are created by first defining the geometry in a data file which is written in a text editor such as notepad, before being imported into Surface Evolver. The data file defines the geometry in terms of vertices (points), edges (vectors), facets (triangles), and bodies (groups of oriented facets). The construction of the models is therefore not a simple task, and care must be taken in order to produce them correctly. Sketching the model initially by hand is strongly recommended to identify all necessary geometry and orientations before proceeding to writing the data file. The data file also contains constraints, and other energies applied to the bodies, as well as any macros defined by the user. Macros can be used to simplify the process of running the models, as well as setting up any post-processing work such as image generation.

C.1.1 *Definition of geometric elements*

Surfaces are defined in Surface Evolver through the use of geometric elements. Each element has its own set of attributes that are defined by the user, or defined internally by the software and can later be queried. A brief overview of each of the geometric elements used to construct a Surface Evolver data file are described below to familiarise the reader with their terminology and function within the model.

Vertices are used to define a point in space by way of a coordinate system. They are used to describe the points on a surface, and their coordinates change as the surface evolves. Vertices of the original surface are defined in the *vertices* section of the data file.

Edges are straight lines that connect two vertices together. Edges can contribute to the surface energy of the system by defining them on a level set constraint or by having named quantity energies applied to them. Edges of the original surface are defined in the *edges* section of the data file.

Facets are oriented faces defined by 3 or more edges. The direction in which the edges are defined determines the orientation of the facet i.e. facing either in or out. By default a facet carries a surface energy equal to its surface area; however the energy can be modified by formula or named quantities. It is recommended to visually check the orientation of each facet by applying the *frontcolor* command to the end of the data file line which will apply the defined colour to only the front oriented face. Facets of the original surface are defined in the *facets* section of the data file.

Bodies are a full-dimensional region of space. They are defined by their boundary of facets or edges, which are used to determine the volume and gravitational energy contributions. Bodies of the original surface are defined in the *bodies* section of the data file.

C.1.2 *Defining variables*

Surface Evolver is able to handle the use of variables and these are defined in the data file header. Variables are declared with the prefix `PARAMETER` and follow the format: `PARAMETER (variable name) = (value)`, where ‘value’ can take the form of an integer, expression, or any previously defined variable.

Setting up the position of the vertices in the data file is a time consuming process and so it is particularly useful to define these positions by using a formula relating to a small number of shared variables. This allows the user to quickly adjust the model simply by changing the variable value, e.g. all vertices on the top of a cube could have a z-axis value equal to the variable ‘cubeheight’.

C.1.3 *Surface tension*

In the physical world one of the main factors governing the shape of the surface of liquid droplets is that of surface tension. This is especially apparent as the physical dimensions decrease and gravitational effects start to become negligible. Surface Evolver assumes the unit less surface tension of a facet to be 1 unless it has been otherwise stated by the user. Each facet may be configured to have a different surface tension. The contribution to the overall surface energy of the system is the facet area multiplied by its surface tension.

C.1.4 *Contact angle*

In the physical world when a liquid makes contact with a solid surface, the liquid-solid interface has its own surface tension (γ_{LS}). This differs from the surface tension of the liquid in contact with the air (γ_{LG}) and must be accounted for during energy calculations. The contact angle is measured at the point where the solid-liquid-air interfaces intersect and is known as the triple contact line (TCL). The liquid-air interface and the liquid-solid interface both pull on the contact line, with the tangential force balance leading to the Equation C-2.

$$(\text{liquid-solid tension}) = -(\text{liquid-air tension}) * \cos \theta \quad (\text{C-2})$$

Where θ is the interior angle the liquid makes with the solid surface measured in radians.

As mentioned in section C.1.3, Surface Evolver automatically sets the tension of any facet to 1 unless specified by the user. To account for the difference in surface tension occurring at the liquid-solid interface the user must set the facet tension at the end of the corresponding line using the TENSION command.

C.1.5 *Volume*

Any bodies that are declared in the data file must also have a volume associated with them. Surface Evolver uses this value when performing its

calculations to determine the size and shape of the surface. As the software deals only in surfaces, the volume for a body is determined by calculating for each facet the volume of the oriented prism between the facet and the $z = 0$ plane. Surface Evolver then sums all the body facet contributions together to determine the overall volume for the body. The orientation of the facet has an effect on how the software calculates the volume, hence vertical faces and those on $z = 0$ plane do not contribute to the body volume. Facets facing upwards have the volume between them and the $z = 0$ plane added to the body volume, whereas those facing downwards have the volume between themselves and the $z = 0$ plane subtracted from the body volume.

The ‘v’ command can be used at the command line to view the *target volume* and *actual volume* of any bodies in the data file at any point during the running of the model. The target volume is the volume that the program is working towards and is the value declared along with the body in the data file. This can be in the form of an integer, or a previously defined variable. The actual volume is the current volume of the body at a given time during the model evolution. This value is calculated as the volume of the body as defined by the vertices, edges and facets in the data file. The target volume is the overriding parameter however and once the model is run Surface Evolver will iterate the geometry to achieve this volume, regardless of the initial volume of the body, set by the geometry of the facets. This is particularly useful as it allows the volume of a body to be easily changed without having to go back and adjust all of the co-ordinate points for the individual vertices.

C.1.6 Constraints

A level-set constraint is used to fix vertices, edges or facets so that they may only exist at a location prescribed by an expression. Typically this is used to force vertices onto the X, Y or Z plane for example so as to allow a droplet to spread across a fixed planar surface. The formula can contain any expression that is known to Surface Evolver or variables that have been previously declared in the data file. Level-set constraints can be defined for equality of inequality, also known as one-sided constraints. The constraint can also have

an energy vector field associated with it that is integrated over edges lying on the constraint. This is useful for defining omitting faces of a body and providing contact angles for liquids intersecting another surface. It is important to note however that integrals are not evaluated along edges which are fixed.

Surface Evolver allows the user to set one-sided constraints which can be used to stop the motion or vertices. A level-set constraint can be specified as either ‘nonnegative’ or ‘nonpositive’, meaning that the vertices must be on one side or the other of the zero level-set. Vertices can move freely during evolution up to the constraint but are not permitted to move into a location that contravenes the constraint. The vertices are free to move back off the constraint if the forces pull them in that direction.

This can be particularly useful to prevent a surface from passing through features of the physical geometry, or from cutting corners during evolution. It can also be used to simulate the boundary between a wettable and non-wettable region on a surface.

C.1.7 *Surface Evolver – Fluid Interface Tool*

Surface Evolver – Fluid Interface Tool (SE-FIT) is a windows based program that features a graphical user interface (GUI) frontend with the Surface Evolver (SE) providing the computational backend. It builds on the existing SE program by moving some of the command line driven features into a more user-friendly GUI. The SE-FIT has been developed at the Capillary Fluidics lab at Portland State University [185]. The program adds a range of pre-built geometries and the ability to perform parametric sweep functions to either compute equilibrium surfaces or to identify surface stability limits in batch mode, which lead to significantly reduced overhead when experimenting with a range of parameters. The software is estimated to offer design efficiencies an order of magnitude higher than current Computational Fluid Dynamics (CFD) packages [186].

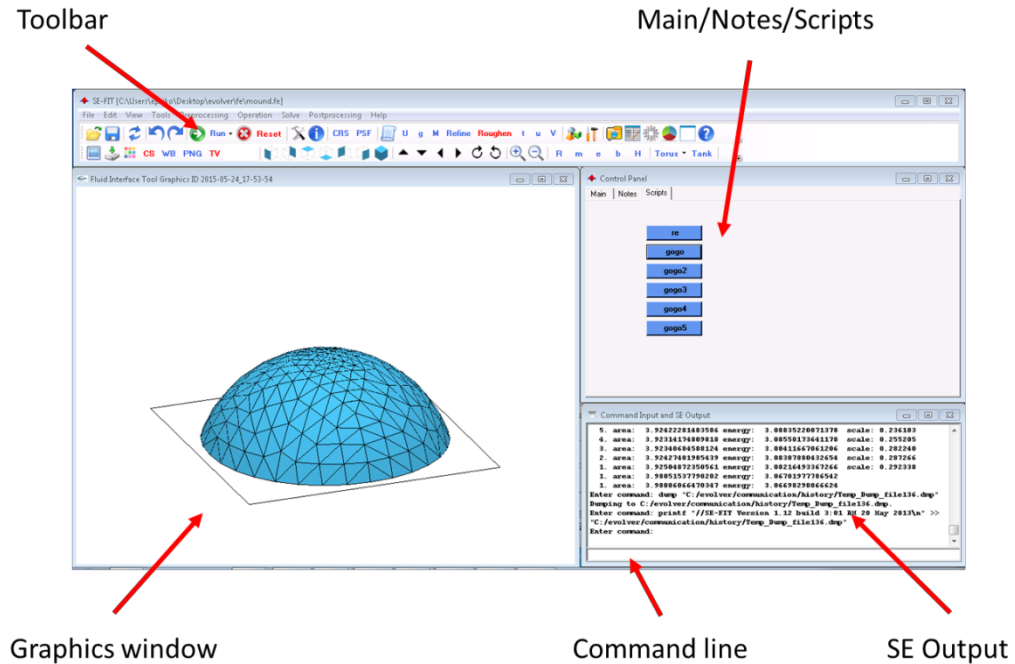


Figure C-1: GUI of SE-FIT software highlighting the main areas of the program.

The GUI of the SE-FIT software (Figure C-1) has been provided above to illustrate the main areas of the program to the reader. The toolbar is home to many of the programs features such as file handling, pre-built geometries, tools, text editor and some graphics manipulation for the graphics window. The graphics window displays the current state of the model and updates in real-time as the data file is computed by Surface Evolver. The upper-right window contains tabs for Main, Notes and Scripts. The ‘Main’ tab contains a list of user-defined parameters that can be edited here without having to change the data file. The ‘Notes’ tab contains any notes that were written in the header of the data file so it is advisable to include a brief description of the model here. Finally the ‘Scripts’ tab contains any macros that were written at the end of the data file and are very useful for automating many functions when running the models. The lower-right window contains the Command line and Surface Evolver output. The command line is used to drive the Surface Evolver software and tell it what computational tasks to carry out such as mesh refinement, iterate etc. Many of the commands are simplified to one-letter, case-sensitive commands for example ‘r’ to refine triangulation of the mesh, ‘g’ to run a single iteration of the model, and ‘i’ to give information on the

current status of the model. A full list of the single letter commands can be found online in the Surface Evolver documentation. The Surface Evolver output window displays the commands being carried out by the software and any computational steps carried out while running the model. For each iteration of the model the output window will display the current iteration number, the interfacial area, the surface energy, and the scale factor.

C.1.8 *Output of results*

Surface Evolver writes everything that appears in the output window to a separate text file. This includes the file name of the data file, a list of any errors detected in the model when the data file is opened, as well as every iteration of the model as it evolves. For each iteration the iteration number, area, surface energy and scale factor are displayed. These are stored locally in the c:\evolver\communication\out folder. Whenever Surface Evolver is opened a new data log is created in the folder with the filename following the naming convention of year-month-day-hour-minute-second. This file is then continuously written to until Surface Evolver is closed. The data displayed in the output window is updated in real time, with only a certain number of lines retained in memory. This means it is necessary to access the output file to view all the iteration steps for a given model. If Surface Evolver is not closed and a new data file is opened, any commands or data appearing in the output window will be written to the same data file. This allows data from multiple data files with varying parameters to be contained within the same output file for later processing.

Having introduced the main concepts of the Surface Evolver software, an example data file is presented in the next subsection to familiarise the reader with their layout.

C.1.9 *Example data file*

Below is an example of a simple data file to familiarise the reader with the layout and notation used to create the models for Surface Evolver. The

example presented is part of the tutorials available on the Surface Evolver website found at <http://www.susqu.edu/brakke/evolver/evolver.html>. This model simulates the evolution of an initial cube. As there are no other forces acting on the cube other than surface tension the cube will evolve to a sphere.

```
// cube.fe
// Evolver data for cube of prescribed volume.

vertices
1  0.0 0.0 0.0
2  1.0 0.0 0.0
3  1.0 1.0 0.0
4  0.0 1.0 0.0
5  0.0 0.0 1.0
6  1.0 0.0 1.0
7  1.0 1.0 1.0
8  0.0 1.0 1.0

edges /* given by endpoints and attribute */
1  1 2
2  2 3
3  3 4
4  4 1
5  5 6
6  6 7
7  7 8
8  8 5
9  1 5
10 2 6
11 3 7
12 4 8

faces /* given by oriented edge loop */
1  1 10 -5 -9 //color red
2  2 11 -6 -10 //color green
3  3 12 -7 -11 //color blue
4  4 9 -8 -12 //color cyan
5  5 6 7 8 //color yellow
6  -4 -3 -2 -1 //color magenta

bodies /* one body, defined by its oriented faces */
1  1 2 3 4 5 6 volume 1
```

It can be seen that this simple data file is split into 5 sections: The header, vertices, edges, faces and bodies. The header contains any notes about the model so it is useful to include the file name and a brief description of the model. For each geometric element the first number in each row denotes the number corresponding to that particular element. For vertices the following three integers are the vertices coordinates in x, y, and z. As previously mentioned these can either be integers or pre-defined variables. Edges are described by defining two vertices, the order of which defines the direction of the edge. Faces are defined by three or more edges and these must connect

head to tail to create a continuous perimeter. The orientation of the edges will determine the final orientation of the face. Bodies are defined by declaring the faces which enclose the body.

C.2 Understanding Surface Evolver

Although tutorials are available to introduce the user to the Surface Evolver software on K.Brakke's website, there is still a steep learning curve to understanding the software and gaining meaningful results. Some of the processes are carried out automatically in the background and are not fully explained to the user such as how calculations are performed for volume and surface energy. This can make it difficult to understand the behaviour of the model when debugging. The following section covers the steps undertaken to understand various aspects of the software and offers advice to new users based on the author's experience and findings.

C.2.1 *Observation on best practice*

As previously mentioned models are constructed through the use of vertices, edges, facets and bodies. The vertices must be defined using a coordinate system, vertices used to define edges, edges to define facets, and finally facets to define bodies. This can quickly become a confusing task if not planned correctly. Drawing a sketch of the wireframe model initially by hand and numbering all vertices and edges can be a huge help when constructing the initial model, particularly for novice users who are unfamiliar with Surface Evolver. Figure C-2 shows a sketch of a basic cube with all vertices and edges numbered sequentially. In this example numbers in circles represent the vertices, and squares for the edges. Arrows indicate the direction in which the edge is defined, i.e. edge 1 is defined as connecting from vertices 1 to vertices 2.

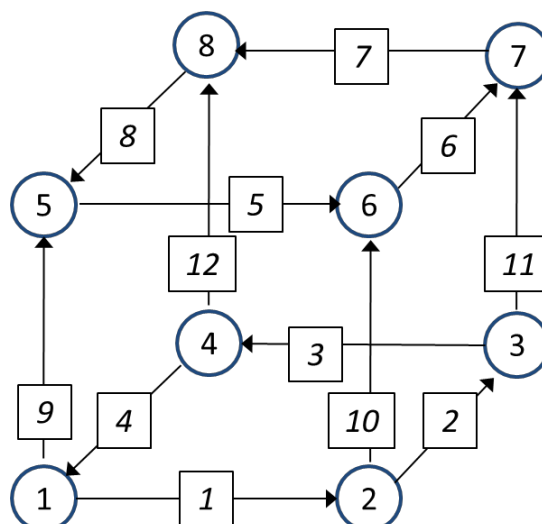


Figure C-2: Sketch of a basic cube model for Surface Evolver labelling vertices and edges. Numbers in circles represent vertices, with numbers in squares representing edges. Arrows indicate the direction in which the edge is defined.

As when writing code for any program it is strongly encouraged to add comments to the end of lines. It is also recommended to add a comments section in the header of the data file describing the purpose of the particular model for later reference.

Edges are defined by two vertices, having a head and tail determined by the order in which the vertices are declared. It is recommended to declare all edges in a consistent manner (i.e. left-right, and down-up) to avoid confusion when later defining the faces.

In order to construct a body correctly, the faces must be declared in a consistent orientation. The edges must form a continuous line around the perimeter of the face, and whether the edge must be declared positive or negative is determined by its previously defined orientation. It is recommended to use the *frontcolor* (*color*) command at the end of the facet declaration which sets the colour of only the front face. This allows the user to visually check the orientation of a face when opening the model. A list of the supported colours can be found in the Surface Evolver documentation.

C.2.2 Surface energy

Surface Evolver calculates the total surface energy of the model by multiplying the surface area of a facet by its surface tension. The surface tension is defined in the data file at the end of the facet line using TENSION (value), where value can be an integer or previously defined variable.

It is important that the user remember to set a surface tension value for all facets as failing to do so results in the software assigning a value of 1. This results in the surface area of the facet being added to the overall total surface energy for the model. If the user is including faces in the model simply for graphical representation e.g. a horizontal plane a surface tension of 0 should be applied, or the perimeter displayed using edges only and given the *bare* command to tell Surface Evolver that they are not being used in the definition of any facets.

Recall from equation (C-2)

), the liquid-solid interfacial energy (γ_{LS}) is equal to the liquid-gas interfacial energy (γ_{LG}) multiplied by the cosine of the contact angle (θ) in radians (Figure C-3).

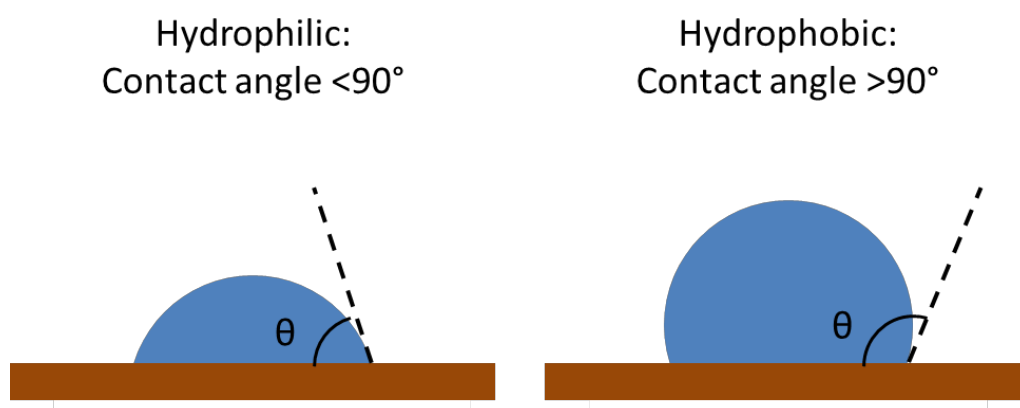


Figure C-3: Diagram illustrating the definition of the contact angle of a liquid droplet on a solid surface.

The range of contact angles for water with surface tension $\gamma = 72.8$ mN/m and the corresponding calculated liquid-solid interfacial energies are summarised in Table C-1.

As was explained in chapter 2, section 2.4.4, the molecules at the interface between the liquid and solid are attracted to the surface by van der Waals forces. In the case of a hydrophilic surface, these attractions are strong and the interfacial energy is negative. Conversely when the surface is hydrophobic, the attractions are weak and the interfacial energy is positive.

Recall that the total energy of the system is equal to the interfacial energy multiplied by the interfacial area ((C-1)). It therefore becomes clear that as the liquid volume is decreased and the meniscus between two solid surfaces becomes smaller, the surface area of liquid in contact with the solid faces become much larger than that of the meniscus in contact with air. In the case of a hydrophilic surface this means that the overall energy of the system will become negative. A negative energy is of course not a physical possibility but recall that Surface Evolver is aiming to solve an energy balance for the lowest possible value and is therefore unconcerned with absolute values.

Contact angle (degrees)	Solid-liquid interfacial energy (mN/m)
0	-72.80
10	-71.69
20	-68.41
30	-63.05
40	-55.77
50	-46.79
60	-36.40
70	-24.90
80	-12.64
90	0.00
100	12.64
110	24.90
120	36.40
130	46.79
140	55.77
150	63.05
160	68.41
170	71.69
180	72.80

Table C-1: Contact angle and corresponding solid-liquid interfacial energy for water, $\gamma = 72.8$ mN/m.

C.2.3 Batch processing

As previously mentioned SE-FIT supports the batch processing of data files. This can be found in Solve>Batch processing. The user needs to specify a folder containing the data files, and provide a set of commands to be used when running the models. SE-FIT then opens and runs each data file in turn, writing to the same output file.

Using the ‘A’ command (case sensitive) provides a numbered list of the model parameters in the output window (and output file). The program expects the user to modify the parameters at this point, so a line containing ENTER is required for the script to proceed. Using the ‘i’ command (case sensitive) provides information on the status of the model. This is a good way to have

the final total surface energy of the model displayed in the output window (and output file).

Due to the large number of data files required it is recommended to batch generate these also using another program. The authors used Matlab to generate the data files for Surface Evolver and to process the results from the produced output file. By using the two one-letter commands mentioned above, the user can identify the correct lines in the output file through markers to extract the necessary data.

A flowchart of the steps followed by the author to create a data set for Surface Evolver simulations is shown in Figure C-4. The two Matlab scripts created for data file generation and post processing of the lateral misalignment case presented in the following chapter can be found in APPENDIX D as an example.

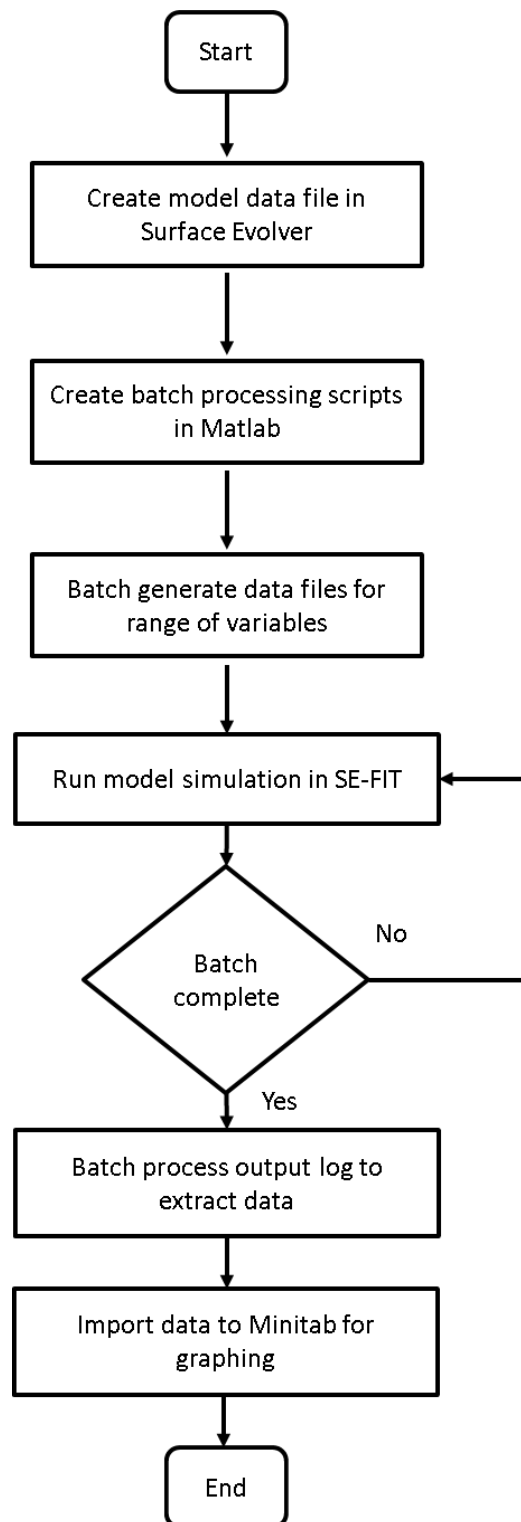


Figure C-4: Flowchart illustrating the steps taken to generate a data set for Surface Evolver simulations.

APPENDIX D - Matlab script for data file generation and post processing

The code presented below is the Matlab script used for the generation of Surface Evolver data files. The example shown here was used for the case of lateral component misalignment in the determination of spring constants.

```

for i=0:100;                                %Set up loop length
x_offset = 0.0005*i;                        %Set increments for offset
* by current loop num
offset = num2str(x_offset);                 %Convert number to string
filename = sprintf('Results_%d.fe', i);     %Set filename based on
loop num
fileID = fopen( filename, 'wt' );           %Open file in write mode
fileA = fopen('fepart1.txt','r');           %Open first part of script
tline = fgetl(fileA);                       %Get all lines from fileA
while ischar(tline)
    fprintf(fileID, '%s\n', tline);          %Print contents into fileID
    tline = fgetl(fileA);
end
fclose(fileA);
fprintf(fileID, '%s\n', offset);             %Add offset value to fileID
fileB = fopen('fepart2.txt','r');           %Open second part of script

tline = fgetl(fileB);                       %Get all lines from fileB
while ischar(tline)
    fprintf(fileID, '%s\n', tline);          %Print contents into fileID
    tline = fgetl(fileB);
end
fclose(fileB);
fclose(fileID);

end

```

```

end

```


This Matlab script was used for the post processing of the data is shown below. This was used to extract the relevant lines from the Surface Evolver output file.

```

fid = fopen('Testout.txt','r');
%Open the SE output log

C = textscan(fid, '%s','Delimiter',' ');
%Scan the document

fclose(fid);

C = C{:};

dataA = ~cellfun(@isempty, strfind(C, '9.          xoffset'));
%Set up search parameters

output = [C{find(dataA)}];
%Find the search term in matrix

columnA = textscan(output, '%*f %*s %f', ' '); %Format the
results to display          number only

dataB = ~cellfun(@isempty, strfind(C, 'Total energy:'));

output2 = [C{find(dataB)}];

columnB = textscan(output2, 'Total energy:%f');

```

APPENDIX E - Surface Evolver Data file

Below is the data file for the Surface Evolver model used in the determination of spring constants. The model was written by K.Brakke and has been adapted to represent the geometries investigated in this thesis.

```
// Surface Evolver model of chip floating on droplet on square pad.

// measurement units: cgs

keep_originals // so numbering in Evolver same as in datafile

// physical
data
gravity_constant 981 // cm/sec^2; much
higher gives fast squishing
parameter TENS = 72.8 // dyne/cm
parameter liquid_density= 1 // g/cm^3
parameter WALLT = (-TENS*cos(70*(pi/180))) //virtual tension

// Key dimensions
// Bottom pad
parameter pad_length = 0.2 // in x-direction, cm
parameter pad_width = 0.2 // in y-direction, cm

// Upper chip
parameter chip_length = 0.2 // in x-direction, cm
parameter chip_width = 0.2 // in y-direction, cm

parameter vol= 0.0005 // initial volume

// Parameters for degrees of freedom of chip.
// These can be made optimizing at run time with the "unfix" command.
// Parameters are all identically zero when chip would be directly on
pads,
// neglecting spacer bump, in perfect alignment.
optimizing_parameter xoffset = 0.0 // offset, cm
optimizing_parameter yoffset = 0.0
optimizing_parameter zoffset = vol/(pad_length*pad_width) // start
optimizing_parameter roll = 0.0 // radians
optimizing_parameter pitch = 0.0
optimizing_parameter yaw = 0.0 // initial twist

scale_limit 1/TENS

// Center of mass, in chip coordinates
//parameter chip_weight = 1.892 // grams (Change
this to mass)**
//parameter chip_cm_x = 0.0 // cm
//parameter chip_cm_y = 0.0 // cm
//parameter chip_cm_z = 0.0250 // cm

// gravitational energy of chip
//quantity chip_grav_energy energy method vertex_scalar_integral
//scalar_integrand: z*G*chip_weight

// 3-parameter "boundary" to define floating chip coordinates,
// copied from the chipx etc formulas above, but angles negated.
```

```

// so angles are positive about axes.
// See Fig_11_2.fe for derivation and further info.
boundary chip_bdry parameters 3
x: (cos(pitch)*cos(yaw)*p1 - cos(pitch)*sin(yaw)*p2 + sin(pitch)*p3 \
    + xoffset)
y: ((sin(roll)*sin(pitch)*cos(yaw)+cos(roll)*sin(yaw))*p1 + \
    (-sin(roll)*sin(pitch)*sin(yaw)+cos(roll)*cos(yaw))*p2
- \
    cos(pitch)*sin(roll)*p3 + yoffset)
z: ((-cos(roll)*sin(pitch)*cos(yaw)+sin(roll)*sin(yaw))*p1 + \
    (cos(roll)*sin(pitch)*sin(yaw)+sin(roll)*cos(yaw))*p2 +
\
    cos(pitch)*cos(roll)*p3 + zoffset)

//
vertices
// Bottom pad
1 -pad_length/2 -pad_width/2 0 fixed
2 pad_length/2 -pad_width/2 0 fixed
3 pad_length/2 pad_width/2 0 fixed
4 -pad_length/2 pad_width/2 0 fixed
// chip, given in parameters p1, p2, p3
5 -chip_length/2 -chip_width/2 0 fixed boundary chip_bdry
6 chip_length/2 -chip_width/2 0 fixed boundary chip_bdry
7 chip_length/2 chip_width/2 0 fixed boundary chip_bdry
8 -chip_length/2 chip_width/2 0 fixed boundary chip_bdry

// the center of mass vertex, in chip parameters p1,p2,p3
//10 chip_cm_x chip_cm_y chip_cm_z boundary chip_bdry fixed
chip_grav_energy

//
edges
// Bottom pad
1 1 2 fixed
2 2 3 fixed
3 3 4 fixed
4 4 1 fixed
// Chip
5 5 6 fixed boundary chip_bdry
6 6 7 fixed boundary chip_bdry
7 7 8 fixed boundary chip_bdry
8 8 5 fixed boundary chip_bdry
// Connecting pad and chip
9 1 5
10 2 6
11 3 7
12 4 8
// Chip
15 5 6 fixed boundary chip_bdry no_refine
16 6 7 fixed boundary chip_bdry no_refine
17 7 8 fixed boundary chip_bdry no_refine
18 8 5 fixed boundary chip_bdry no_refine
// Bottom pad
21 1 2 fixed no_refine
22 2 3 fixed no_refine
23 3 4 fixed no_refine
24 4 1 fixed no_refine

//
faces
1 21 22 23 24 fixed color brown no_refine
// pad
2 15 16 17 18 fixed color yellow boundary chip_bdry no_refine
// chip
3 1 10 -5 -9 tension TENS color lightblue
4 2 11 -6 -10 tension TENS color lightblue

```

```

5   3 12 -7 -11 tension TENS color lightblue
6   4  9 -8 -12 tension TENS color lightblue

//_____
bodies
1  -1 2 3 4 5 6 density liquid_density volume vol

//_____

// Twist offset evolution
Twist_offset := { set background white ; fix roll ; fix yaw ; fix
pitch ;
    r; r; refine edge where original >= 1 and original <= 8;
    { g 10 ; V 2; u } 20 ; r ; refine edge where original >= 1 and
original <= 8;
    { g 10 ; V ; u } 5 ;
    { g 10 ; V ; u } 100;
}

// X-offset evolution
x_offset := { set background white ; fix roll ; fix yaw ; fix pitch ;
fix xoffset ; fix zoffset;
    r; r; refine edge where original >= 1 and original <= 8;
    { g 10 ; V 2; u } 20 ; r ; refine edge where original >= 1 and
original <= 8;
    { g 10 ; V ; u } 50 ;
}

// Z-offset evolution
z_offset := { set background white ; fix roll ; fix yaw ; fix pitch ;
    r; r; refine edge where original >= 1 and original <= 8;
    { g 10 ; V 2; u } 20 ; r ; refine edge where original >= 1 and
original <= 8;
    { g 10 ; V ; u } 5 ;
    { g 10 ; V ; u } 100;
}

// Tipping angle evolution
tipping_angle := { set background white ; fix roll ; fix yaw ; fix
pitch ; fix zoffset ;
    r; r; refine edge where original >= 1 and original <= 8;
    { g 10 ; V 2; u } 20 ; r ; refine edge where original >= 1 and
original <= 8;
    { g 10 ; V ; u } 5 ;
    { g 10 ; V ; u } 100;
}

// Droplet misalignment evolution
Drop_mis := { set background white ; fix roll ; fix yaw ; fix pitch ;
fix xoffset ; fix yoffset ;
    r; r; refine edge where original >= 1 and original <= 8;
    { g 10 ; V 2; u } 20 ; r ; refine edge where original >= 1 and
original <= 8;
    { g 10 ; V ; u } 100;
}

```

APPENDIX F - Matlab script for differentiation of surface energy

The code presented below is the Matlab script used for the differentiation of Surface Evolver derived surface energy to establish force generated by the liquid droplet. The example shown here was used for the case of lateral component misalignment in the determination of spring constants.

```

xx = linspace(0.0,0.0005);                                %Sets up range for x-axis
pp = spline(columnA,columnB);                               %creates spline of the 2
data sets
[breaks,coefs,l,k,d] = unmkpp(pp);                         %Extract data from piece-
wise-polynomial
pp2 = mkpp(breaks,repmat(k-1:-1:1,d*1,1).*coefs(:,1:k-1),d);
      %make the derivative
plot(xx,ppval(pp2,xx),'-r')                                % plot the derivative of the
polynomial
h = findobj(gca,'Type','line')
x=get(h,'Xdata')
y=get(h,'Ydata')
x=x';
y=y';
fit = polyfit(x,y,8);                                       % fit the data with an 8th
order polynomial
newy = polyval(fit,xx);
plot (xx,newy);                                             % plot the new data
h = findobj(gca,'Type','line')
x=get(h,'Xdata')                                           % extract x values from
plotted data
y=get(h,'Ydata')                                           % extract y values from
plotted data
x=x';
y=y';

```

APPENDIX G– Analytical solution of combined lateral misalignment case

This solution simplifies the model geometry to that of a parallelepiped, with the liquid interface being represented as straight sides. The model assumes that the bottom face of the component remains parallel to the top surface of the binding site, and that there is no relative twist in the orientation of the component and binding site at any time.

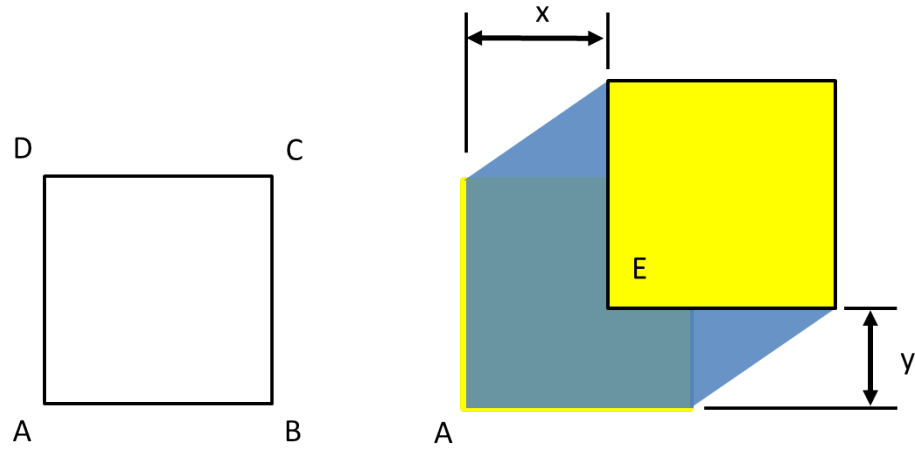


Figure G-1: Diagram illustrating the definition of the model elements and component misalignment.

The length of the droplet edge is calculated based on the component misalignment:

$$AC = \sqrt{x^2 + y^2} \quad (G-1)$$

$$AE = \sqrt{x^2 + y^2 + h^2} \quad (G-2)$$

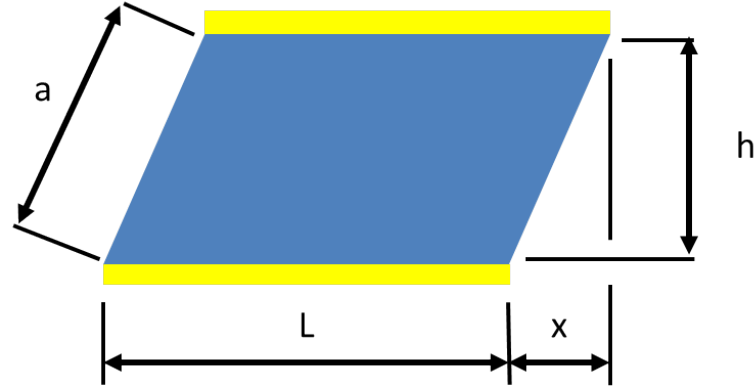


Figure G-2: Diagram of the component under combined lateral misalignment when viewed normal to one of the side planes of the component/binding site.

Considering the observed shift in a single plane:

$$h = \sqrt{a^2 - x^2} \quad (\text{G-3})$$

$$h_2 = \sqrt{a^2 - x^2} \quad (\text{G-4})$$

This leads to the total interfacial area for the two matching x-sides:

$$\begin{aligned} S_x &= 2L\sqrt{a^2 - x^2} \\ &= 2L\sqrt{x^2 + y^2 + h^2 - x^2} \quad (\text{G-5}) \\ &= 2L\sqrt{y^2 + h^2} \end{aligned}$$

With the interfacial area of the two matching y-sides being:

$$S_y = 2L\sqrt{a^2 - y^2} \quad (\text{G-6})$$

$$= 2L\sqrt{x^2 + y^2 + h^2 - y^2}$$

$$= 2L\sqrt{x^2 + h^2}$$

The total surface energy of the liquid-air interface can therefore be shown to be:

$$E = 2\gamma L \left(\sqrt{y^2 + h^2} + \sqrt{x^2 + h^2} \right) \quad (\text{G-7})$$

APPENDIX H- Analytical solution of vertical displacement case

The solution assumes that the component has an equilibrium position when placed on a liquid droplet. When the component is moved down the droplet is compressed and forms a convex profile. When the component is lifted up the droplet is stretched and forms a concave profile. The interface is simplified to assume that each face has a circular profile (Figure H-1).

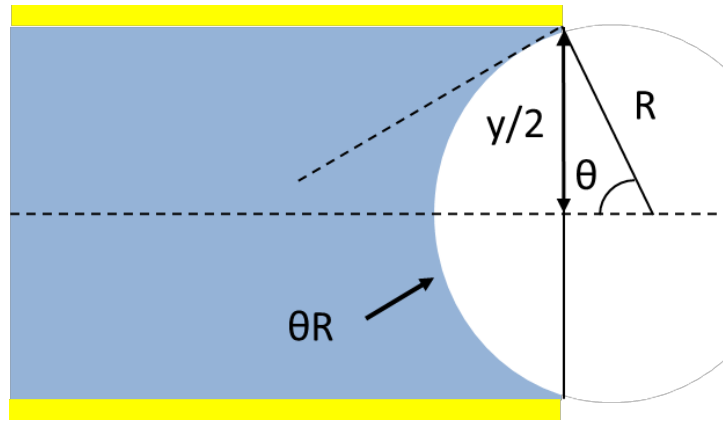


Figure H-1: Diagram of circular interface for liquid droplet under vertical component displacement.

The total interfacial area can be expressed as:

$$S = 4L(2\theta R) \quad (H-1)$$

With the constant droplet volume being:

$$V = L^2 h_0 = L^2 y - 4L \left(\theta R^2 - \frac{y}{2} R \cos \theta \right) \quad (H-2)$$

Using the relation

$$R = \frac{y}{2 \sin \theta} \quad (H-3)$$

Leads to:

$$L^2 h_0 = L^2 y - L \frac{y^2}{\sin \theta} \left(\frac{\theta}{\sin \theta} - \cos \theta \right) \quad (\text{H-4})$$

$$\text{for } -\frac{\pi}{2} > 0 > \frac{\pi}{2}$$

For a given angle θ , y is a quadratic polynomial

$$y = \frac{L \pm L \sqrt{1 + 4 \frac{1}{\sin \theta} \left(\frac{\theta}{\sin \theta} - \cos \theta \right) \frac{h_0}{L}}}{\frac{2}{\sin \theta} \left(\frac{\theta}{\sin \theta} - \cos \theta \right)} \quad (\text{H-5})$$

APPENDIX I - Surface Evolver data file for modelling curved edges

The Surface Evolver data file presented below was created to investigate the effect of curved edge on a square binding site and how these influenced the surface energy of a liquid droplet.

```
//Onesidedcurvededge.fe
//Model to examine the effect of a liquid droplet passing over a
//curved edge.
//The droplet is pinned to the edges and only has 1 curved edge.
//Component is in a fixed position and liquid volume varied.

gravity_constant 981 // gravity cm/s^2
parameter TENS = 72.8
parameter vol = 0.00038
parameter RR = 0.0005 //radius of edge
parameter pad = 0.2 //dimension of binding site
parameter zheight = 0.01 //height of binding site
parameter zoffset = 0.00875 //initial height of component
parameter xoffset = 0.0 //initial misalignment of
component
parameter undercut = 90 //angle of edge geometry
parameter slope = (180-undercut)*(pi/180) //angle of sidewall in
radians
parameter slope2 = ((undercut*(pi/180))/2) //half of sidewall angle
parameter curvang = 90*(pi/180) //angle of arc along curved
edge
//centres of upper circle
parameter circ1top1 = RR/(tan(slope2)) //x,y coordinate for upper
circles
parameter circ1top2 = pad-circ1top1 //x,y coordinate for opposite
end of pad
parameter circ1top3 = -RR //z coordinate for upper
circles
parameter basex = zheight/(tan(slope)) //position of binding site
base
parameter topx = RR/(tan(slope2)) //intersect of radius with top
surface
parameter bottomx = tan(slope2)*RR //interect of raidus with
bottom of "trench"
parameter sidey = (sin(slope)*RR) //interect of radius with
sidewall (x,y)
parameter sidez = (cos(slope)*RR) //interect of radius with
sidewall (z)
parameter zcurve = (cos(curvang)*RR) //initial z-position of
droplet on curved edge
parameter xcurve = (sin(curvang)*RR) //initial x-position of
droplet on curved edge
parameter angle = 70 //contact angle of
liquid with solid (degrees)
parameter dropslide = 0.0
parameter compdens = 0.946
parameter compheight = 0.05
parameter component_mass = (pad^2)*compheight*compdens

#define WALLT (-TENS*cos(angle*(pi/180))) //virtual tension

scale_limit 1/TENS // scale limit in convergence
process
```

```

keep_originals // keep initial numbers for
vertices

// gravitational energy of component
quantity component_grav_energy energy method vertex_scalar_integral
scalar_integrand: z*G*component_mass

//
constraint 1 //level set constraint for
binding site top surface
formula: z = 0

constraint 2 CONVEX //Constraint describing the
circular edge
formula: (y-circtop1)^2+(z-circtop3)^2=RR^2

constraint 3
formula: x = 0

constraint 4
formula: x = pad

constraint 5 //constraint for component
position
formula: z = zoffset

constraint 6 nonnegative //non-negative constraint to
prevent liquid shortcutting curve geometry
formula: (y-circtop1)^2+(z-circtop3)^2=RR^2

constraint 7 nonpositive
formula: y = 0

constraint 8 nonpositive
formula: z = zoffset

constraint 9 nonnegative
formula: z = 0

//
vertices
//binding site top surface
1 0 topx 0 fixed constraint 1
2 pad topx 0 fixed constraint 1
3 pad pad-droptop 0 fixed constraint 1
4 0 pad-droptop 0 fixed constraint 1

//top of sidewall
5 0 circtop1-sidez circtop3+sidez fixed
6 pad circtop1-sidez circtop3+sidez fixed

//bottom of sidewall
7 0 -basez -zheight fixed
8 pad -basez -zheight fixed

//component
9 0 0-xoffset zoffset fixed constraint 5
10 pad 0-xoffset zoffset fixed constraint 5
11 pad pad-xoffset zoffset fixed constraint 5
12 0 pad-xoffset zoffset fixed constraint 5

//droplet intersect with curved edge
13 0 circtop1-xcurve circtop3+zcurve constraint 2 6 fixed
14 pad circtop1-xcurve circtop3+zcurve constraint 2 6 fixed

```

```

//component centre of mass
15 pad/2 (pad/2)-xoffset zoffset+(compheight/2) fixed
component_grav_energy

//
edges
//binding site
1 1 2 fixed constraint 1 no_refine
2 2 3 fixed constraint 1 no_refine
3 3 4 fixed constraint 1 no_refine
4 4 1 fixed constraint 1 no_refine

//sidewall
5 5 6 fixed
6 7 8 fixed no_refine
//sidewall verticals
7 7 5 fixed no_refine
8 8 6 fixed no_refine

//curved edge
9 5 1 constraint 2 3 6
10 6 2 constraint 2 4 6

//component
11 9 10 fixed no_refine constraint 5
12 10 11 fixed no_refine constraint 5
13 11 12 fixed no_refine constraint 5
14 12 9 fixed no_refine constraint 5

//liquid brdige
15 1 9
16 2 10
17 3 11
18 4 12

//droplet intersect with curved edge
19 13 14 constraint 2 6 fixed

//droplet intersect with curved edge verticals
20 13 1 constraint 2 3 6 fixed
21 14 2 constraint 2 4 6 fixed

//liquid bridge between droplet on curve and component
22 13 9
23 14 10

//
facet
//binding site
//1 1 2 3 4 frontcolor yellow constraint 1 fixed no_refine

//curved edge
//2 5 10 -1 -9 frontcolor yellow constraint 2 tension 0

//sidewall
//3 6 8 -5 -7 frontcolor yellow fixed no_refine

//droplet base
4 -1 -4 -3 -2 frontcolor yellow tension WALLT constraint 1 fixed
no_refine

//droplet sidewalls
5 19 23 -11 -22 frontcolor lightblue tension TENS constraint 6
6 2 17 -12 -16 frontcolor lightblue tension TENS constraint 8 9
7 3 18 -13 -17 frontcolor lightblue tension TENS constraint 8 9

```

```

8 4 15 -14 -18 frontcolor lightblue tension TENS constraint 8 9

//droplet top
9 11 12 13 14 frontcolor green tension WALLT constraint 5 fixed
no_refine

//component
//10 11 12 13 14 frontcolor green constraint 5 no_refine

//droplet on curved edge
11 -19 20 1 -21 frontcolor yellow tension WALLT constraint 2 6 fixed
no_refine

//additiional droplet sidewalls
12 21 16 -23 frontcolor lightblue tension TENS constraint 6
13 -20 22 -15 frontcolor lightblue tension TENS constraint 6

//_____

bodies
1 4 5 6 7 8 9 11 12 13 volume vol density 1

//_____

read

Run := {{r; g; }3; u; V; r; g 100; u; V; g 100; }

Run2 := {
  r; refine edge where original >= 1 and original <= 8;
  { g 10 ; V 2; u } 20 ; r ; refine edge where original >= 1 and
original <= 8;
  r; g 10; u; V;
  { g 100 ; V ; u } 10; }

valuecheck := { convert_to_quantities; show_all_quantities; Q; }

```

APPENDIX J - Surface Evolver data file for modelling undercut structures

The Surface Evolver data file presented below was created to investigate the effect of undercutting the square binding site and how this influenced the surface energy of a liquid droplet.

```
//Undercut_structures.fe
//Model to examine the effect of a liquid droplet moving down binding
//site sidewall.
//The droplet is pinned to the edges and only has 1 undercut edge.
//Component is held in a fixed position and liquid volume varied.

gravity_constant 981 // gravity
parameter TENS = 72.8 //Surface tension
parameter vol = 0.00036 //volume of liquid
parameter angle = 70 //contact angle of
liquid
parameter RR = 0.0005 //radius of edge
parameter pad = 0.2 //dimension of binding site
parameter zheight = 0.01 //height of binding site
parameter zoffset = 0.00875 //initial height of
component
parameter undercut = 90 //angle of edge geometry
parameter slope = (180-undercut)*(pi/180) //angle of sidewall in
radians
parameter basex = zheight/(tan(slope)) //position of binding site
base
parameter factor = 1 //loop number
parameter dropmod = factor*0.0005
parameter arcstepx = dropmod*cos(slope) //modified droplet position on
sidewall
parameter arcstepz = dropmod*sin(slope)
parameter grad = zheight/basex //gradient of sidewall
parameter compdens = 0.946
parameter compheight = 0.05
parameter component_mass = (pad^2)*compheight*compdens

#define WALLT (-TENS*cos(angle*(pi/180))) //virtual tension

scale_limit 1/TENS // scale limit in convergence
process
keep_originals // keep initial numbers for
vertices

// gravitational energy of component
quantity component_grav_energy energy method vertex_scalar_integral
scalar_integrand: z*G*component_mass

constraint 1
formula : z = 0

constraint 2 nonnegative
formula : z = 0

constraint 3
formula : z=grad*y

//_____

vertices
//droplet base
1 0 0 0 fixed constraint 1
```

```

2 pad 0 0 fixed constraint 1
3 pad pad 0 fixed constraint 1
4 0 pad 0 fixed constraint 1

//sidewall
5 0 -basex -zheight fixed
6 pad -basex -zheight fixed

//component
7 0 0 zoffset fixed
8 pad 0 zoffset fixed
9 pad pad zoffset fixed
10 0 pad zoffset fixed

//droplet sidewall
//11 0 0 -dropmod fixed constraint 3
//12 pad 0 -dropmod fixed constraint 3
11 0 -arcstepx -arcstepz fixed
12 pad -arcstepx -arcstepz fixed

//droplet extensions to avoid zero area
13 0 -0.001 zoffset/2
14 pad -0.001 zoffset/2

//component centre of mass
15 pad/2 pad/2 zoffset+(compheight/2) fixed component_grav_energy

//

```

```

edges
//base
1 1 2 fixed constraint 1
2 2 3 fixed constraint 1
3 3 4 fixed constraint 1
4 4 1 fixed constraint 1

//sidewall verticals
5 5 1 fixed no_refine
6 6 2 fixed no_refine

//sidewall
7 5 6 fixed no_refine

//component
8 7 8 fixed no_refine
9 8 9 fixed no_refine
10 9 10 fixed no_refine
11 10 7 fixed no_refine

//liquid bridge
12 1 7
13 2 8
14 3 9
15 4 10

//droplet sidewall
16 11 12 fixed constraint 3

//droplet sidewall verticals
17 11 1 fixed constraint 3
18 12 2 fixed constraint 3

//droplet extension
19 13 14

//droplet extension verticals
20 11 13
21 12 14

```



```

22 13 7
23 14 8

//_____

faces
//droplet base
1 -1 -4 -3 -2 frontcolor yellow tension WALLT constraint 1 no_refine

//component
2 8 9 10 11 frontcolor yellow tension WALLT fixed no_refine

//droplet
//3 1 13 -8 -12 frontcolor lightblue tension TENS
4 2 14 -9 -13 frontcolor lightblue tension TENS
5 3 15 -10 -14 frontcolor lightblue tension TENS
6 4 12 -11 -15 frontcolor lightblue tension TENS

//droplet sidewall
7 -16 17 1 -18 frontcolor yellow tension WALLT fixed no_refine
constraint 3

//droplet extension faces
8 19 23 -8 -22 frontcolor lightblue tension TENS
9 16 21 -19 -20 frontcolor lightblue tension TENS
10 20 22 -12 -17 frontcolor lightblue tension TENS
11 18 13 -23 -21 frontcolor lightblue tension TENS

//_____

bodies
1 1 2 4 5 6 7 8 9 10 11 volume vol density 1

//_____

read

Run2 := {
  r; refine edge where original >= 1 and original <= 8;
  { g 10 ; V 2; u } 20 ; r ; refine edge where original >= 1 and
original <= 8;
  r; g 10; u; V;
  { g 10 ; V ; u } 200; }

valuecheck := { convert_to_quantities; show_all_quantities; Q; }

```

APPENDIX K - Surface Evolver data file for micro component test case

The Surface Evolver data file presented below was created to investigate a micro component test case of a high aspect ratio structure assembled onto a square binding site.

```
//Tippingmodel.fe
//model to simulate the tipping of a tall square-based structure
//model pivots about one edge and liquid volume varied

//units: CGS

gravity_constant 981 //gravity cm/s^2
parameter TENS = 72.8 //surface tension of liquid-
air interface
parameter pad = 0.2 //length of pad edge
parameter zoffset = 0.0 //initial height of component
corner
parameter tilt = 6.5 //angle of component tilt in
degrees
parameter compx = cos(tilt*(pi/180))*pad //x-component for
component position
parameter compz = sin(tilt*(pi/180))*pad //z-component for
component position
parameter grad = compz/compx
parameter vol = 0.0003
parameter WALLT = -cos(70*(pi/180))*TENS
parameter droptslide = 0.001 //distance droplet de-
pinned from edge
parameter factor = 45 //model iteration
parameter dropmod = droptslide*factor
parameter dropcompx = cos(tilt*(pi/180))*(pad-dropmod)
parameter dropcompz = sin(tilt*(pi/180))*(pad-dropmod)
parameter compdens = 0.946 //component density g/cm
parameter comp_height = 11 //height of component in z-
axis cm
parameter theta = atan((comp_height/2)/(pad/2))
//angle to component centre radians
parameter comphyp = sqrt(((comp_height/2)^2)+((pad/2)^2))
//hypotenuse to component centre cm
parameter component_mass = (pad^2)*comp_height*compdens
//component mass grams

// gravitational energy of component
//quantity component_grav_energy energy method vertex_scalar_integral
//scalar_integrand: z*G*component_mass

constraint 1 //constraint for bottom face
formula: z = 0

constraint 2 nonpositive //constraint for tilt
formula: z = grad*y

constraint 3 nonnegative
formula: z = 0

constraint 4 nonpositive
formula x = pad

constraint 5 nonnegative
formula x = 0

//-----
```

```

vertices
1 0 0 0 fixed
2 pad 0 0 fixed
3 pad pad 0 fixed
4 0 pad 0 fixed

//5 0 0 zoffset fixed
//6 pad 0 zoffset fixed
7 pad compx zoffset+compz fixed
8 0 compx zoffset+compz fixed

//droplet de-pinned vertices
9 pad pad-dropmod 0 fixed
10 0 pad-dropmod 0 fixed
11 pad dropcompx dropcompz fixed
12 0 dropcompx dropcompz fixed

//modification for droplet liquid bridge
//to prevent excessive changes in shape
13 pad pad-(dropmod/2) compz/2 constraint 2 3 //4 5
14 0 pad-(dropmod/2) compz/2 constraint 2 3 //4 5

//component centre of mass
//15 pad/2 cos(theta+(tilt*(pi/180)))*comphyp
sin(theta+(tilt*(pi/180)))*comphyp fixed component_grav_energy

//-----

edges
//binding site
1 1 2 fixed no_refine
2 2 3 fixed no_refine bare
3 3 4 fixed no_refine bare
4 4 1 fixed no_refine bare

//component
5 2 7 fixed no_refine bare
6 7 8 fixed no_refine bare
7 8 1 fixed no_refine bare

//liquid droplet
9 2 9 color red fixed
10 9 10 color red fixed
11 10 1 color red fixed

12 2 11 color red fixed
13 11 12 color red fixed
14 12 1 color red fixed

//liquid bridge
15 9 13 constraint 2 3
16 10 14 constraint 2 3
17 13 11 constraint 2 3
18 14 12 constraint 2 3

//liquid bridge halfway point
19 13 14 constraint 2 3

//-----

faces
1 -1 -11 -10 -9 frontcolor yellow fixed no_refine tension WALLT
constraint 3
2 1 12 13 14 frontcolor green fixed no_refine tension WALLT constraint
2

```

```

//liquid bridge
3 9 15 17 -12 frontcolor lightblue tension TENS constraint 2 3
4 10 16 -19 -15 frontcolor lightblue tension TENS constraint 2 3
5 11 -14 -18 -16 frontcolor lightblue tension TENS constraint 2 3
6 19 18 - 13 -17 frontcolor lightblue tension TENS constraint 2 3

//-----

bodies
1 1 2 3 4 5 6 density 1 volume vol

//-----

Read

Run := { g; r; g5; r; g10; r; g 200;
        u; V;
        g 100; r;
        u; V;
        g 100;
        }

Run2 := {
        r; refine edge where original >= 1 and original <= 8;
        { g 10 ; V 2; u } 20 ; r ; refine edge where original >= 1 and
original <= 8;
        r; g 10; u; V;
        { g 10 ; V ; u } 50; }

```