TOWARDS OPTIMAL DESIGNS FOR SELF-ALIGNMENT IN SURFACE TENSION DRIVEN MICRO-ASSEMBLY

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ABSTRACT

Fluidic self-assembly driven by surface tension force has demonstrated the capability of assembling micro parts to binding sites in parallel with high efficiency and accuracy. In this paper, we focus on the binding site design for this technique, as it is a critical factor not only for accurate assembly, but also to achieve *unique alignment position and orientation*. To find optimal designs, we use a first-order approximation model to evaluate a series of patterns including disks, rings and offset rings. From this analysis, optimal patterns assuring unique alignment are determined to be offset rings with specific geometric constraints. For comparison, experiments with different shapes are performed, and results matching with the simulations are observed.

1. INTRODUCTION

Micro-assembly provides parallel integration of devices produced from different, possibly incompatible processes [e.g., 1-4]. Self-assembly using surface tension as driving force has been shown to provide accurate positioning between parts and binding sites [2,3]. For example, when a Au patterned substrate is soaked in an alkane-thiol SAM (self-assembled monolayer) solution, a monolayer forms only on Au, creating a hydrophobic region on a surrounding hydrophilic SiO_2 background. Hydrocarbon lubricant forms exclusively on these hydrophobic regions when the substrate is immersed in water. Introduced devices patterned with Au attach to the lubricant and are assembled on binding sites by the surface tension force of the lubricant. This approach resembles annealing, with the final assembly representing a minimum energy state.

Although good positioning has been reliably achieved, the challenging problem of how to optimize the geometric shape of parts and binding sites, in particular to achieve *unique orientation and alignment* for asymmetric devices such as diodes, or to maximize yield, has remained open. As a first solution, we employ a series of part designs and study their behavior during a surface tension driven self-assembly process. Matching simulation and experimental results show how their design parameters can be chosen to obtain precise positioning as well as unique orientation, which is required for alignment of devices for which polarity is important.

The broader goal of this work is to create a general foundation and techniques to understand and optimize surface tension driven self-assembling microsystems.

2. MODEL AND SIMULATION

During self-assembly of a part to a binding site, a certain surface energy W associated with its relative position and orientation, is influenced by the shape of the hydrophobic binding site and the liquid meniscus of the lubricant, as well as material properties. The assembly force is given as the gradient of this energy $F = \nabla W$. Finite element methods (FEM) such as, e.g., Surface Evolver are common modeling tools to calculate surface tension forces and energies, and give accurate but computationally expensive results [5]. This paper addresses the more difficult "reverse" problem of determining binding site designs that optimize the driving forces for accurate and unique assembly. To accomplish this task, we calculate and compare the assembly forces for a series of designs and then select the best available patterns.

More efficient modeling tools are important to analyze large numbers of designs. Previous research introduced a linear model of surface energy derived from the overlap area of part and binding site [4,6], and showed that this approximation is adequate as long as the lubricant thickness is smaller than the misalignment distance [5].

Here, our simulation uses this model to generate *energy and force profiles* in order to describe the dynamics of the self-alignment process while the part approaches the binding site. An energy (resp., force) profile assigns an energy value (resp., force/torque vector) to each part placement relative to the binding site, specified by (x,y,θ). Dynamic simulation of the part can be determined from the energy profile with a gradient descent method that describes its motion as placements with successively lower surface energy (Fig. 1).

It was found that most designs lead to non-unique alignment with at least two distinct energy minima. For example, squares have shown accurate but *non-unique positioning* with four possible orientations [5]. Similarly, disks have good position accuracy but *no preference in orientation*. Rings, i.e. disks with circular cutouts, exhibit local minima when their rims overlap, but these minima become less significant with decreasing cutout hole size, and disappear at a threshold value, leaving only one global minimum.

Thus, the cutout ratio r/R, i.e. the ratio of inner and outer radius, is a *design parameter* that influences the self-assembly behavior. Rings are rotationally symmetric, and thus cannot lead to unique orientation during self-assembly. Therefore, we introduce a second design parameter by adding an offset d between the disk center and cutout center. In the remainder of this paper, we analyze the effect of these two parameters on the self-assembly behavior of offset rings.

3. DESIGN OPTIMIZATION

In our search for designs with unique alignment, ring-shaped patterns with circular cutouts are investigated. Patterns are determined by two parameters, r/R and d/R, where r represents the radius of the cutout, R represents the disk radius and d represents the offset between disk and cutout center. For all shapes, we calculate the surface energy as a function of translation (x,y) between part and binding site (Figs. 2, 3a, 4a) or a function of orientation θ (Fig. 4b). Analytically, concentric rings ($d = 0$) with r/R below a threshold ratio (calculated as ≈ 0.45) have only one energy

minimum, corresponding to exact alignment (Fig. 2c). Experimentally, this is confirmed with rings showing alignment for r/R = 0.3, and rings with r/R = 0.5 and 0.8 stuck in misalignment (Fig. 1). Furthermore, force analysis shows that wide rings (r small generate stronger forces than disks (r = 0) when close to exact alignment (Fig. 3b).

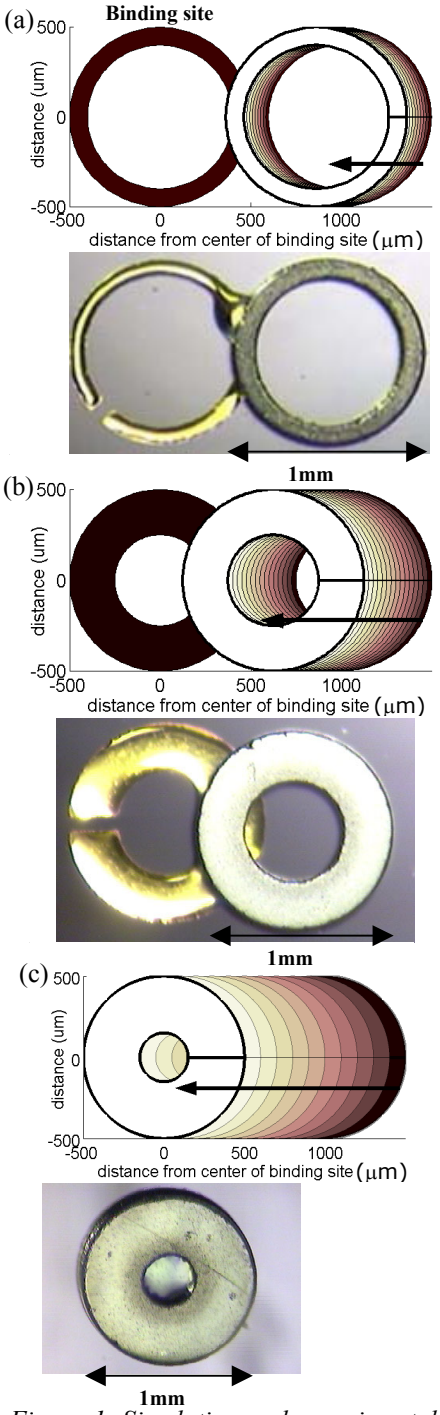

Figure 1. Simulation and experimental results agree on the locations of local energy minima during self-assembly of ring-shaped parts. They get stuck at those positions for cutout ratios (a) r/R = 0.8 and (b) r/R = 0.5. With further decreased cutout ratio (c) r/R = 0.3, only one global minimum remains, where part and binding site exactly align.

Shifting the cutout-center away from the disk-center (d > 0) creates asymmetry, and a unique energy minimum not only appears in translation, but also in rotation (Fig. 4). Further simulation shows the motion of parts starting from the right (Fig. 5a) and left (Fig. 5b) of the binding site until alignment is achieved.

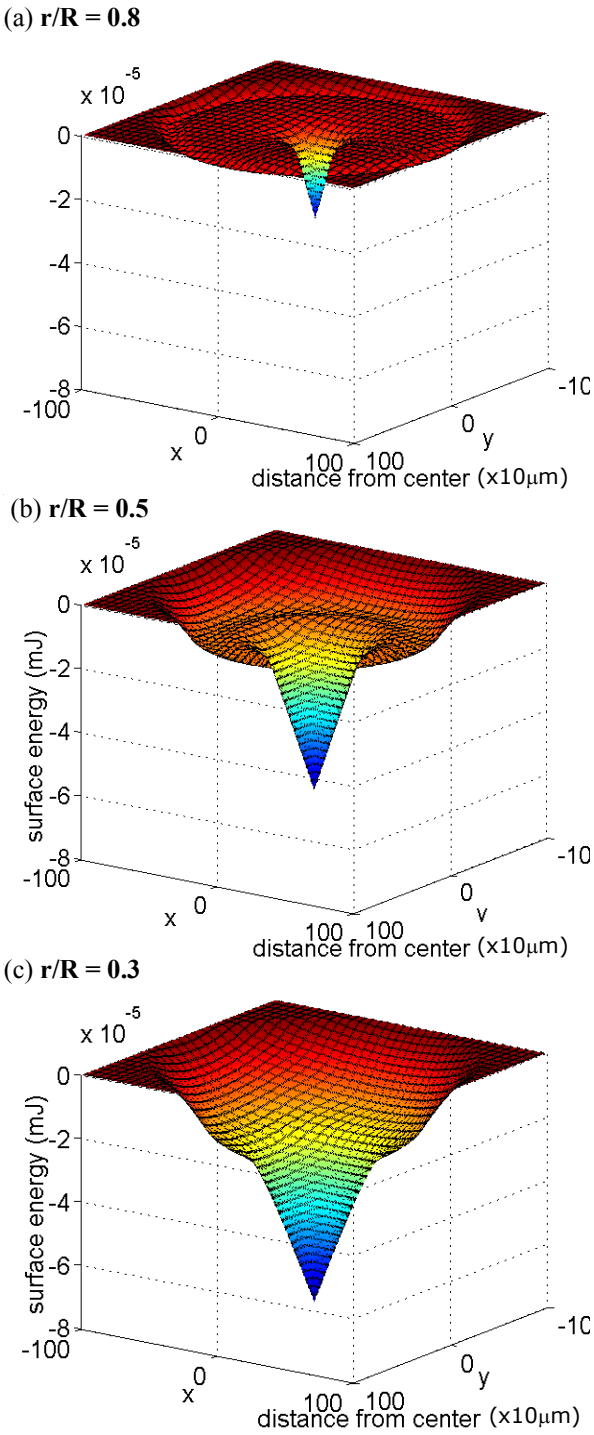

Figure 2. Translation energy profiles show surface energy as a function of relative part position for rings with different cutout ratios r/R. Energy is minimized with exact alignment. Other local minima exist for (a) r/R = 0.8 and (b) r/R = 0.5, but not for (c) r/R = 0.3.

4. Experimental Setup

Parts are produced by cutting a 200µm thin Si wafer with a 355nm wavelength laser (ESI) followed by KOH removal of accumulated particles along cut lines, TiW/Au sputtering, and release in a sonicator.

Substrates are coated with Cr/Au, lithographically patterned and soaked in ethanolic dodecane-thiol solution to form hydrophobic SAM on the binding sites. Then, heat-curable lubricant (triethylene glycol dimethacrylate 97wt.% and benzoyl peroxide 3wt.%) is applied to the substrate and attracted to SAM-coated sites when the substrate is immersed in water. A 20µm wide gap is created in the pattern to prevent lubricant from covering the whole pattern including the cutout part [7] (Fig. 1). Finally, parts are introduced and the self-assembly process is observed under a microscope.

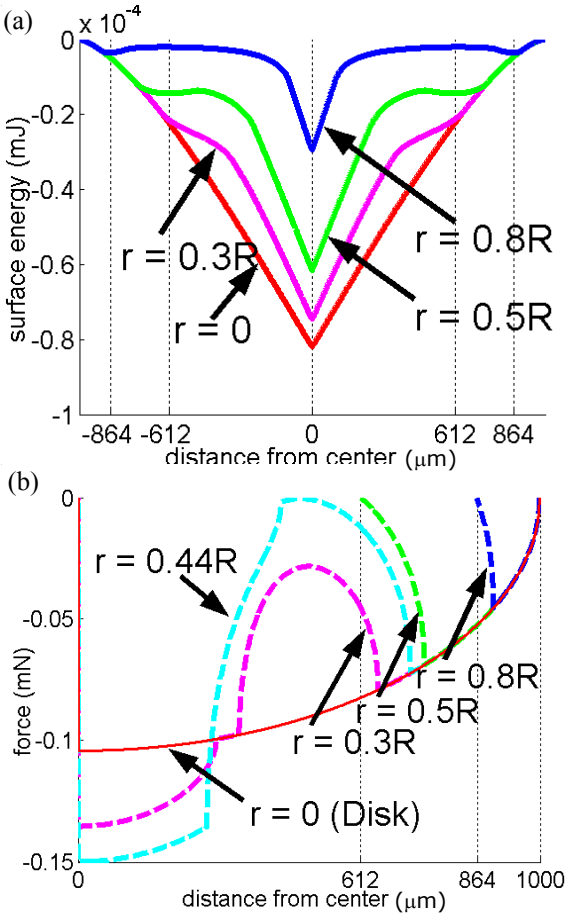

Figure 3. (a) Energy profiles: For ratios of r/R = 0.5 and 0.8 local minima exist at distance ±610µm and ±860µm, respectively. (b) The corresponding force profiles show that when r/R ≥ 0.45, the force vanishes before the part reaches alignment, and it can get stuck without reaching correct alignment.

5. Results and Conclusions

In agreement between simulation and experiments, ring-shaped designs show good alignment for small values of *r*/*R* and misalignment for larger *r*/*R* (Figs. 1-3). For example, rings designed with parameters (*R*, *r*/*R*, *d*/*R*) = (500µm, 0.4, 0.24) show alignment in position and orientation between part and binding site (Fig. 4).

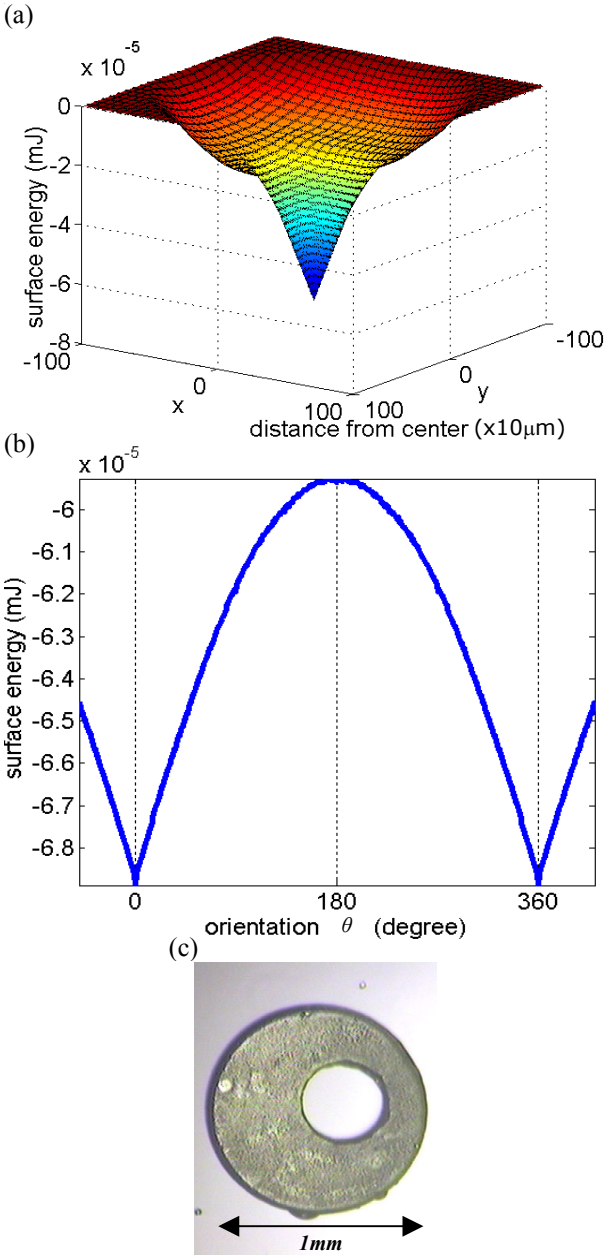

Figure 4. Energy profiles for offset ring design with (R, r/R, d/R) = (500µm, 0.4, 0.24). (a) A global minimum of surface energy is found at (x,y)=(0,0) while translating the part over the binding site. (b) The global minimum also appears when part orients with the binding site for (x,y)=(0,0). (c) Experimental result shows exact alignment of the silicon part over the SAM-coated gold binding site in water.

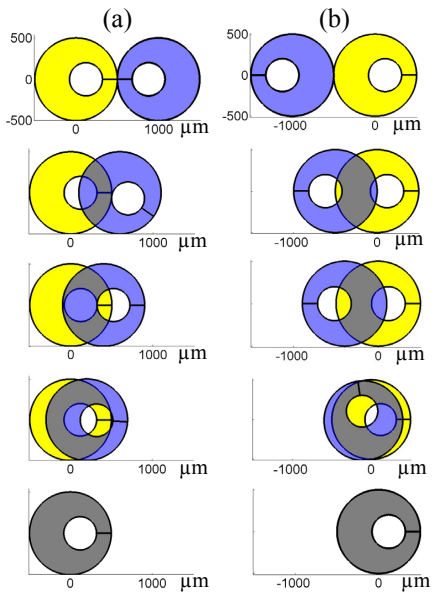

Figure 5. Dynamic simulation snapshots: With the initial position (dark/blue) of the part at either side of the binding site (light/yellow), the part aligns with the binding site due to continuous surface tension force.
(a) (x, y, θ) = (999, 0, 180°) → (0,0,0).
(b) (x, y, θ) = (-999, 0, 180°) → (0,0,0).

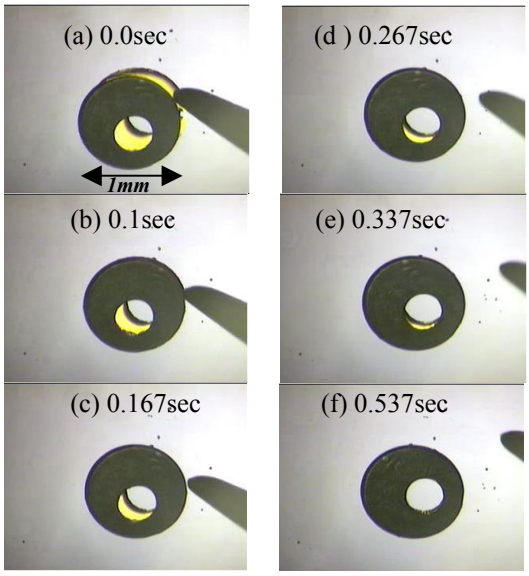

Figure 6. This sequence of video frames shows how the part was able to shift and rotate back from the misalignment situation. Tweezers were used to force the part away from the binding site to observe the process of self-alignment.

One global minimum both in translation and rotation is found from these results. The video sequence shows translation and rotation from a certain misalignment back to exact alignment (Fig. 6).
It is found that translation occurs before rotation due to the significantly larger energy gradient during shifting of the part. A matching path route is obtained from simulation (Fig. 7).

In summary, our work presents (1) a model for the dynamics of surface-tension driven self-assembly, (2) good agreement between simulation and experimental results with a series of designs, (3) shape optimization to achieve *unique position and orientation*, (4) results that are helpful to improve self-assembly yield, which will be studied in more detail in future work.

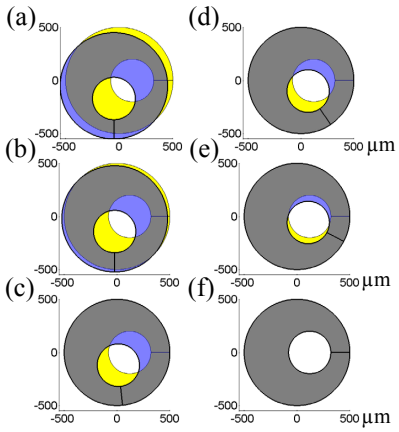

Figure 7. Dynamic simulation with initial placement set as (x, y, θ) = (-50, -50, 270°) → (0,0,0°). Translation of the part takes place before rotation begins.

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