Capillary Forces in Micro-Fluidic Self-Assembly

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ABSTRACT

Parallel self-assembly in the fluidic phase is a promising alternative technique to conventional pick-and-place assembly. In this work the hydrophobic-hydrophilic material system between binding sites for microparts is simulated with respect to alignment precision. The results are compared with experimental findings and allow predictions for the optimization of the fluidic self assembly technique.

Keywords: fluidic self assembly, hybrid integration

1 INTRODUCTION

State of the art microengineering includes a wide range of methods that allow for massive downscaling of components and single devices with functionalities in different energy domains, as e.g. optics, electronics, and fluidics. Material incompatibilities often encountered in monolithic integration require efficient microassembly methods [1] for hybrid systems. Using capillary forces for self-assembly has been proven to be a promising candidate for this need [2], where microparts are packaged on binding sites. The key issue is the control of hydrophobic and hydrophilic surfaces of binding sites and microparts. Many different questions arise regarding accuracy goals for self-assembly in the fluidic phase. The binding site and micropart shape is of crucial significance for the uniqueness of assembling and has been investigated in detail [3].

Moreover, the strengths of the capillary forces and the potential energy shape with respect to the degrees of freedom are crucial for an eventual accurate alignment. To accelerate detection of optimized fluidic systems parameters for self-assembly it is essential to apply simulations to different configurations in order to reduce extensive experimental effort.

One specific observation from the simulation of the fluidic system is that the existing potential energy minimum will always result in a force or torque softening. Accurate alignment thus is improved by reducing the quadratic part in the potential energy which is achieved by reduction of the lubricant volume.
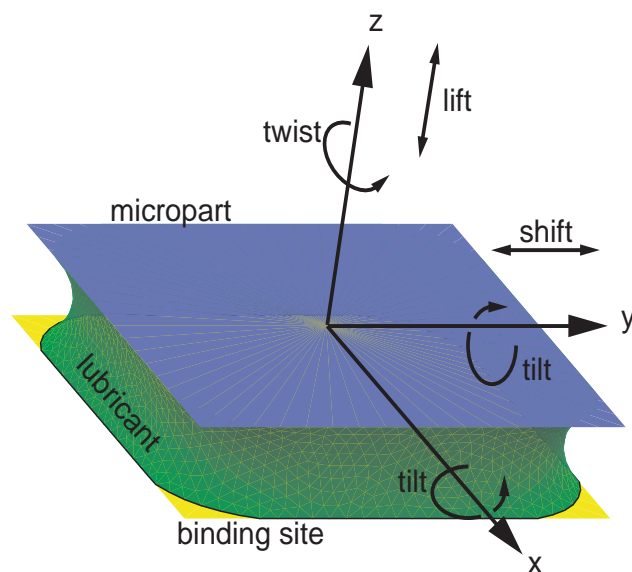

Fig. 1: Geometry. The part displacements, with respect to the substrate pad, are measured using a local coordinate frame. The shape of the liquid meniscus was computed numerically.

2 SIMULATIONS

The simulated system consists of square shaped binding sites and microparts with exactly the same dimensions. In the experimental setup the binding sites are coated with a hydrophobic alkanethiol layer (a self-assembled monolayer, or SAM), and a lubricant liquid is applied to the binding sites while the entire system is immersed in water. Lubricant droplets of well controlled volume form on the binding sites. The microparts are coated with the same SAM and are attracted by the lubricant sitting on the binding part due to capillary forces. The surface energies of the water-lubricant interface

(46 mJ/m^2) and the coating-water interface (52 mJ/m^2) show similar values, while the lubricant-coated interface (< 1 mJ/m^2) is of 2 orders of magnitude less [3]. This difference of nearly two orders of magnitude in the surface energies is the driving force that assures self-alignment.

In our simulations we calculated the total surface energies for different configurations with the *surface evolver* software by K. A. Brakke [4]. The potential energy for various displacements of the micropart relative to the binding site and for different lubricant volumes was calculated. These displacements are schematically reproduced in Fig. 1. They include a shift of the micropart against the binding site, a lift of the micropart in the direction perpendicular to the binding site, a twist rotation with the rotation axes taken as the z-axes, and a tilt motion, i.e a rotation with respect to an axes in the plane of the micropart. Different lubricant volumes have been investigated. There is a clear dependence of the final alignment precision on the variations in the alignment forces and corresponding potential field.
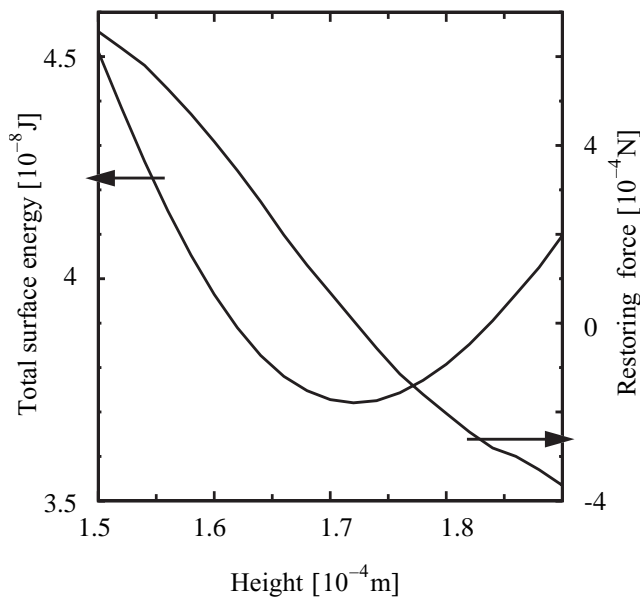
3 RESULTS

Fig. 2: Lift displacement potential energy (left scale) and restoring force (right scale).

In Fig. 2 the potential energy with respect to a displacement of the micropart perpendicular to the binding site surface is drawn. The amount of lubricant volume corresponds to 200 nl. The minimum energy is found at a distance of 0.174 mm between the binding site and the micropart. The system is rather stiff against lift displacement.

For the tilt displacement of the micropart the potential energy and restoring force is shown in Fig. 3. A rapid increase is detected already for small tilt angles and thus a good parallel alignment of the micropart and the binding site is expected.
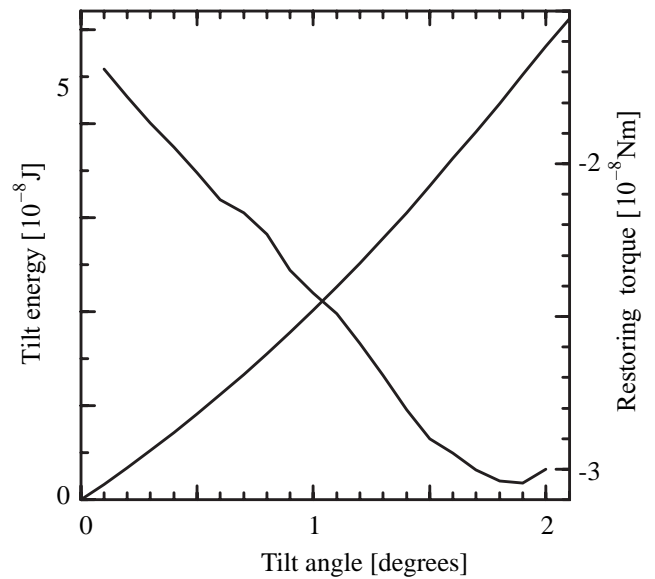

Fig. 3: Tilt displacement potential energy (left scale) and restoring force (right scale).
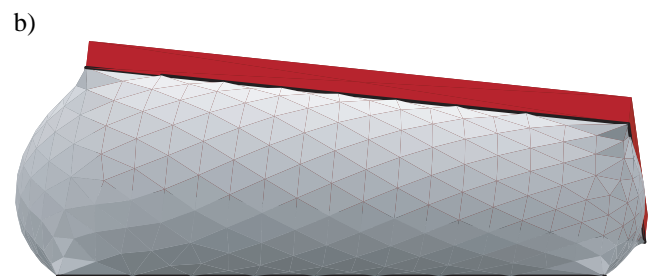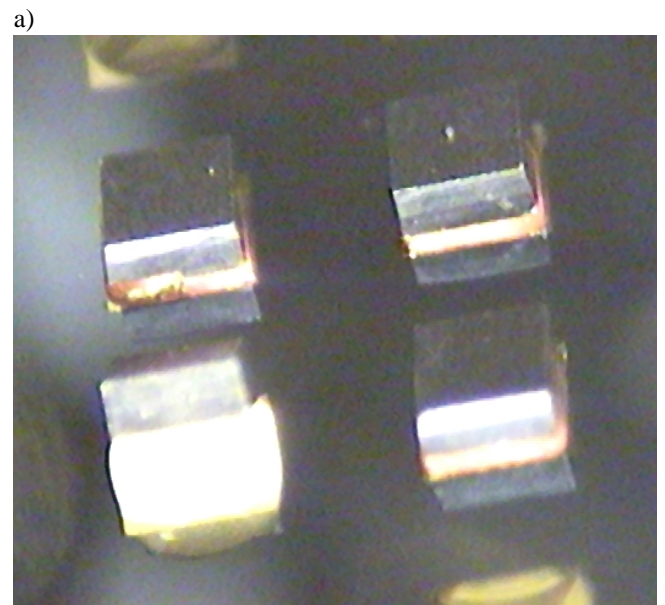
a)

b)

Fig. 4: Increased lubricant volume a) experiment and b) simmulation.

This situation changes dramatically when the amount of lubricant is uncontrollably high. The experimental situation is demonstrated in Fig. 4 a). On a single binding site of parallel assembled microparts an exceedingly high amount of lubricant of about 500 nl was deposited which is roughly ten times the volume used in the aligned micropart shown in Fig. 4 a). The micropart-lubricant system shows a tilt deformation due to the increased liquid volume.

This behavior is reproduced in the simulation where a minimum tilted energy configuration is detected due to arising misaligned potential energy minima with increased lubricant amount. In Fig. 4 b) the result of a quasi-static time integration is shown. The system is considered highly damped, i.e. no inertial effects are present. This enforces the detection of possible local energy minima that become more apparent under these circumstances. For the time integration an Euler method was used with the forces f and torques τ calculated by the principle of virtual work [4]. This results in changes of the rotation angle $\Delta\phi$ and changes of shifts $\Delta r = (\Delta x, \Delta y, \Delta z)$ according to

$$\Delta\phi = \frac{1}{2}\frac{\tau_\phi}{I_\phi}\Delta t^2 \tag{1}$$

$$\Delta r = \frac{1}{2}\frac{f}{m}\Delta t^2 \tag{2}$$

respectively, where τ_ϕ is the torque component and I_ϕ its respective moment of inertia. After each timestep forces and torques are recalculated according to the new position. Three angular degrees of freedom and the shift displacements are used (see Fig. 1).
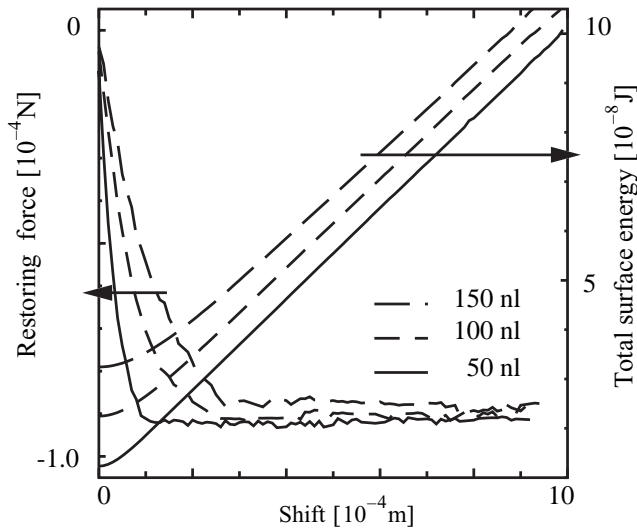

Fig. 5: Shift potential energy (right scale) and saturating restoring force (left scale)

Fig. 5 shows the potential energy as a function of shift misalignment between micropart and binding site. The restoring

force for three different lubricant volumes is shown. The potential minimum lies at the position of perfect alignment. By increasing the shift the restoring force first increases linearly and then saturates to a constant value for large displacements. The slope of this increase is higher the lower the lubricant volume is. In addition the final saturation level is higher for lower lubricant volume.

The constant force was already predicted in [3]. Fig. 6 shows the potential energy and restoring torque due to a twist displacement. Both results clearly show that for increasing amount of lubricant an alignment force/torque softening arises. This corresponds with experimental observations given in Figs. 7a-c on $1\,\text{mm}^2$ square microparts and binding sites. The final alignment is the better the less lubricant is used. Initial effects hampering the alignment may be overcome by external perturbations.
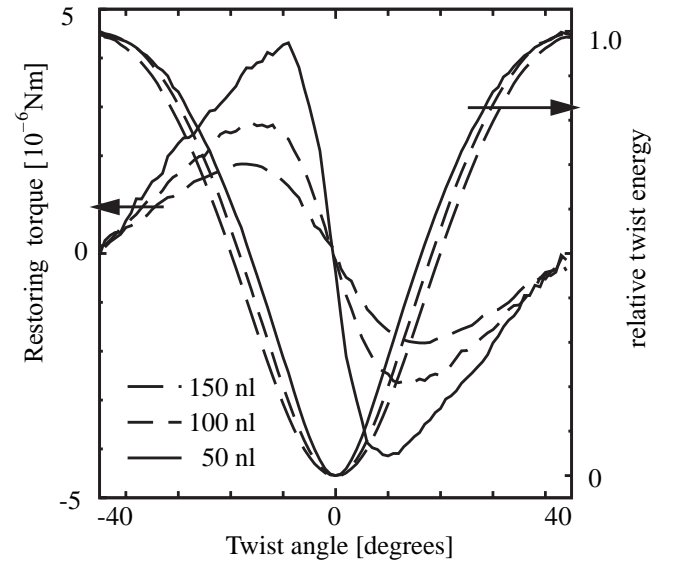

Fig. 6: Relative twist potential energy as a function of twist angle (right scale) $\Phi(\varphi) = (E(\varphi) - E(0))/(E(45°) - E(0°))$ and restoring torque (left scale).

This clearly indicates that the weak forces and torques are due to a quadratic potential for small displacements. Therefore slight imperfections may result in local minima at misaligned states that are more stable the more lubricant is used.

4 SUMMARY AND CONCLUSION

We calculated the surface energy of a self-assembling system in the liquid phase. The emerging restoring forces due to displacements of the microparts were calculated. Both, experiment and simulation show that lift displacements and tilts are detected to be rather uncritical unless the amount of lubricant is exceedingly high. The system turns out to be rather stiff with respect to such displacements.

As expected, a more critical behavior arises from shift and twist displacements. The quadratic increase in surface energy for shift and twist displacements results in a decrease of the
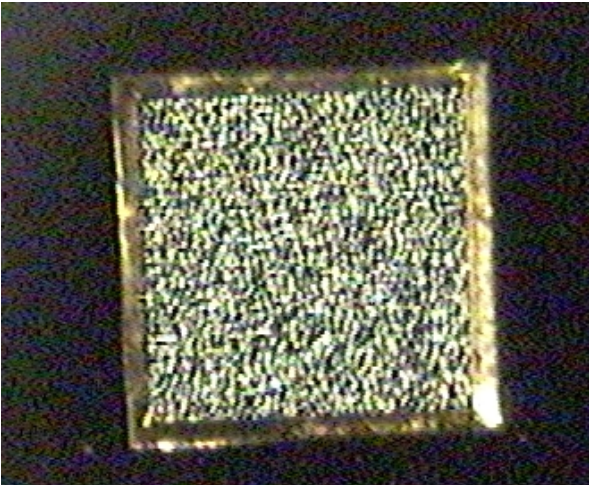
a)
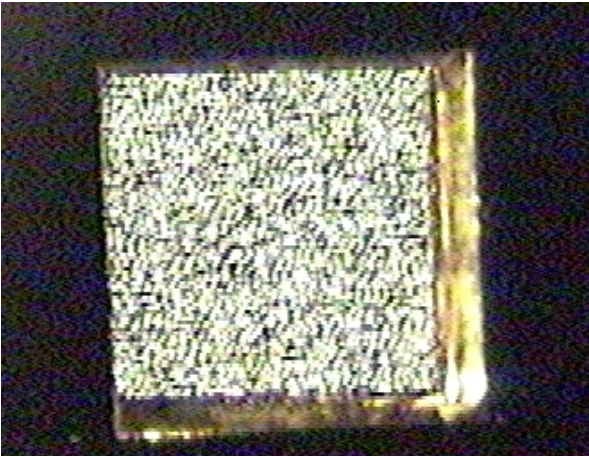
b)

c)

Fig. 7: Aligned Micropart, top view (cf. Fig. 1, viewed in negative z-direction) of a) assembled micropart, misaligned, b) external perturbation, c) and realignment after perturbation.

restoring force and the restoring torque near the point of perfect alignment.

To reduce this restoring force softening a reduction of the lubricant volume must be performed. The reduction of a factor three for an already low lubricant amount of 150 nl increases the stiffness of the system remarkably, i.e. the increase of restoring forces and torques is higher the less lubricant is present. Slight imperfections may nevertheless cause local minima and prevent from a final parallel alignment of the binding site edges and the edges of the micropart. This results in a trade-off between technologically feasible lubricant volume control and acceptable design variations.

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