Simulation of the Dynamic Behaviour of a Droplet on a Structured Surface using the Non-conservative Level Set Method

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Abstract: The ongoing trend towards miniaturization, higher integration as well as towards more cost efficiency will make it necessary to investigate a new assembly method for micro components. In this paper a novel method of fluidic-based micro assembly is presented. A selfassembly effect which is caused by the predominant surface tension and structured surfaces is used to position droplets and to align microchips. Results from numerical analysis and simulations were evaluated and completed by experiments made in cooperation between the IFF-MST University of Stuttgart and the Fraunhofer IPA.

Keywords: Selfassembly, Microassembly, Microfluidic, Level Set Method, Multi-Phase flow.

1. Introduction

Regarding electronic components there is an ongoing trend towards miniaturization and higher integration as well as towards more cost efficiency. The conventional manufacturing methods for microchips based on pick-and-place will reach their limits concerning accuracy of positioning, throughput and handling of micro components. A new technology for assembling very small objects will be necessary. A method based on selfassembly will form a key technology for the realization of future micro production. For future microchips which are smaller than 500 µm we therefore propose a novel assembly technology based on the use of fluids and microfluidic effects. As a driving force for movement and assembly this fluidic-based technology will use the forces caused by the surface tension which is predominant in the micro scale.

2. Principle

In principle this method uses forces based on the predominant microfluidic effect, caused by the surface tension. In microfluidics the surface forces prevail against volume forces and are high enough to grip and move micro objects to a well defined position [1]. That means in the micro scale there are forces caused by the surface tension which can be used as driving forces for assembling micro components. Therefore the process is based on using a surface with hydrophilic (more wetting or water loving) and hydrophobic (less wetting) areas and the influences of structured interfaces on microfluidics [2]. It is possible to position droplets and to move microchips to specified positions for assembly by using well defined hydrophilic and hydrophobic areas on the surface of the substrate [3].

For the fluidic-based microassembly method the surface is structured with well defined hydrophobic and hydrophilic areas as shown in Figure 1. First a droplet (catching droplet) with a diameter of about 200 µm is positioned in the middle of a well defined hydrophobic ring on the substrate. The hydrophobic ring highlights the proper position for the catching droplet and keeps the droplet inside the ring. The inner diameter of this ring is 200 µm. For making electrical contact there are two contact droplets with a conductive fluid which are applied in the same way.

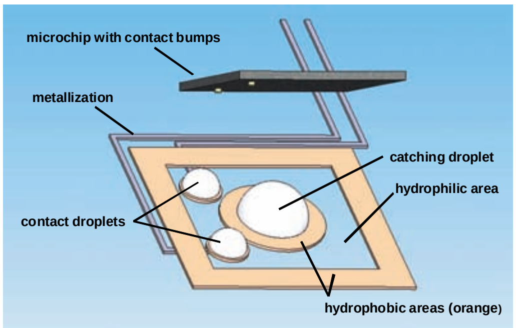

Figure 1: Principle method for fluidic-based assembly of microchips.

After the deposition of the droplets on the substrate the microchip (here its length is 500 µm) will be applied on top of the catching droplet. The task of the selective addressed catching droplet (which is surrounded by a hydrophobic ring in the middle in Figure 1) is to catch the microchip and to place this microchip in the correct assembly position. Therefore the catching droplet will override the hydrophobic ring by use of capillary forces which are caused by the hydrophilic surface of the deposited microchip. The hydrophobic rectangle (Figure 1) is a barrier for the fluid and marks the final position for alignment of the microchip. The movement and positioning of the droplet and the microchip to their final position is a result of the surface tension of the fluid and the minimization of the surface energy in thermodynamic equilibrium.

3. Comsol Multiphysics

The simulation of the dynamic behaviour of a droplet on a structured substrate surrounded by a gaseous environment is done with a multiphase model which takes wetted walls into account. This model has the capability to track the fluid-fluid interface and to describe changes in physical properties such as density, viscosity, contact angle etc. The non-conservative level set method [4] is used as the computation method for solving these problems. The level set method is based on continuum approach in order to represent surface tension and local curvature at the interface as a body force. This allows capturing any topological changes due to changes in surface tensions. In this method the interface between two phases is represented by a smooth function, called level set function Φ(r, t). The level set function is always positive in the continuous phase and is always negative in the dispersed phase. The interface is implicitly represented by the points where the level set function is zero. From such a representation of an interface we can calculate the motion of the free surface by advection of the level set function:

$$\frac{\partial \Phi}{\partial t} + \mathbf{u}\nabla\Phi = \gamma\nabla\left[\epsilon\nabla\Phi - \Phi(1-\Phi)\bullet\mathbf{n}\right] \tag{1}$$

The governing equations of motion for the incompressible isothermal flow can be written in terms of the Navier-Stokes equation which is the equation for the fluid velocity u and pressure p [5]. The Navier-Stokes equation describes the balance of force densities f_{type} acting on fluid elements:

$$\varrho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\nabla)\mathbf{u}\right] = f_{press} + f_{frict} + f_{vol} \tag{2}$$

The body force density f_{vol} includes gravitational force and the surface tension term due to the level set treatment of interfacial stresses. The f_{vol} term is represented by the two components:

$$f_{volx} = \sigma\cdot\kappa\cdot\frac{\partial\Phi}{\partial x}\cdot\delta(\Phi) \qquad f_{voly} = \sigma\cdot\kappa\cdot\frac{\partial\Phi}{\partial y}\cdot\delta(\Phi) + \rho\cdot g \tag{3}$$

The surface tension term at the interface which is determined by the position of the zero level set is treated by the delta function δ (Φ). The curvature κ of the fluidic interface is represented in terms of level set function:

$$\kappa = \nabla\mathbf{n} \tag{4}$$

The unit vector n on the interface points from dispersed phase to continuous phase. In terms of the level set function the unit vector can be described as:

$$\mathbf{n} = \frac{\nabla\Phi}{|\nabla\Phi|} \tag{5}$$

The change in physical properties is described by the Heavyside function which is represented in terms of level set function:

$$H(\Phi<0)=0 \qquad H(\Phi=0)=\frac{1}{2} \qquad H(\Phi>0)=1 \tag{6}$$

Density and viscosity which are constant in each fluid are represented in terms of Heavyside function as:

$$\rho = H(\Phi) + \frac{\rho_{discret}}{\rho_{continous}}(1-H(\Phi)) \qquad \eta = H(\Phi) + \frac{\eta_{discret}}{\eta_{continous}}(1-H(\Phi)) \tag{7}$$

The set of non-linear equations are solved in "COMSOL Multiphysics" by using the finite element method [5] and the direct solver UMFPACK.

4. Simulation results

The positioning of a droplet to a well defined area was studied by numerical simulations. To reduce the computational time we assume a 2D multiphase model. Figure 2 shows the 2D simulation results of a falling droplet (red) on the functionalized surface (orange and green). It is a cross-section of the substrate shown in Figure 1. The hydrophobic ring is in orange and the hydrophilic areas are in green.

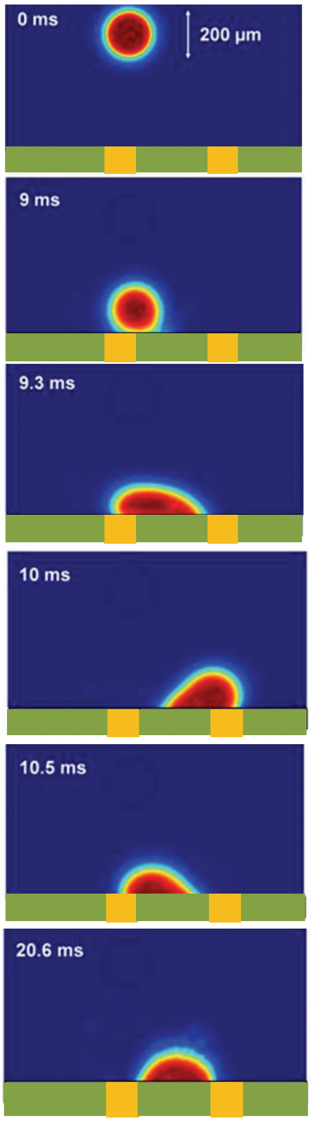

Figure 2: Simulation of droplet positioning.

The catching droplet is dispensed with an initial displacement to its final position. The droplet hits the surface at the interface between the hydrophilic and hydrophobic area (picture at 9 ms in Figure 2). After the droplet hits the substrate and has full contact to the surface it moves in the direction of the hydrophilic surface (picture at 9.3 ms in Figure 2). Reaching the right hydrophobic area, the droplet will overshoot the hydrophobic area because of its mass inertia (Figure 2, picture at 10 ms). The acceleration of the droplet is again in direction of the hydrophilic array. The droplet will slow down and move back into the other direction. After about 10 damped oscillations the droplet has a stable position and nearly zero displacement to its target position (picture at 20.6 ms in Figure 2).

The mean velocity of the interface of the moving droplet on the substrate is about 0.2 m/s and the maximum occurring speed is about 2 m/s.

Figure 3 shows the time depending development of the amplitude when the droplet is overriding the hydrophobic barrier on the substrate (Figure 2, overriding of orange areas). The positive values of the amplitude correspond to the overriding of the left hydrophobic barrier and the negative values to the overriding of the right barrier.

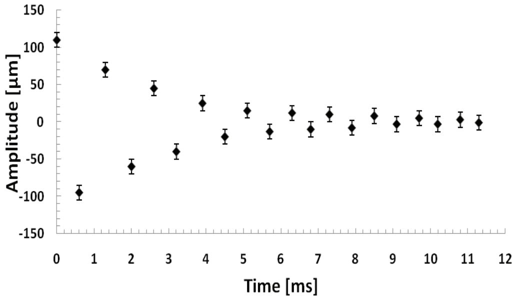

Figure 3: Amplitude when overriding barrier.

The development of the values is characteristically for a damped oscillation. The oscillation frequency is about 840 Hz.

From full contacting the surface (picture at 9.3 ms in Figure 2) until the final position of the droplet (picture at 20.6 ms in Figure 2) it needs about 11.3 ms. At this time the remaining displacement (Figure 3, amplitude at t=11.3 ms) is about 1 µm and therefore negligible. Now the droplet is placed fully to its target position on the hydrophilic area and is ready for the following assembly step which is the catching of the microchip.

Additionally the time for positioning of a droplet depending on the initial displacement was calculated by a number of simulations. Because of the high number and complexity of the transient analysis the numerical simulations were stopped when there was a remaining displacement of about 15%. Figure 4 shows simulation results for calculating the necessary time for positioning of a droplet with a diameter of 200 µm to a well defined area with a remaining displacement of about 15% depending on its initial displacement.

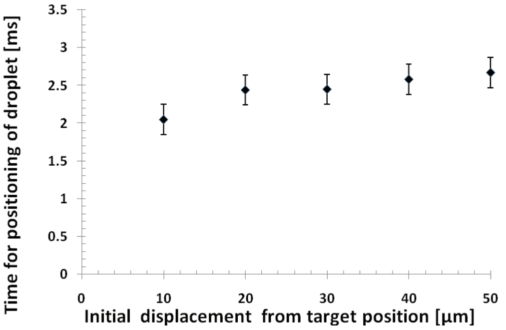

Figure 4: Time for positioning of a droplet.

The comparison of these results shows that the time for positioning of the droplet is increasing with its initial displacement. In general there is a slight accretion of the time for positioning a droplet depending on the initial displacement. In additional we can say this time is in the range of some milliseconds.

Since for positioning of the catching droplet a hydrophobic barrier (see Figure 1, ring) is necessary a number of simulations to determine the width of the hydrophobic ring were made. The dimension of this ring is depending on the initial displacement of the dispensed droplet. The initial displacement of the droplet from its target position was varied and the amplitude when overriding the barrier was calculated by separate simulations. The results of the numerical simulations are shown in Figure 5.

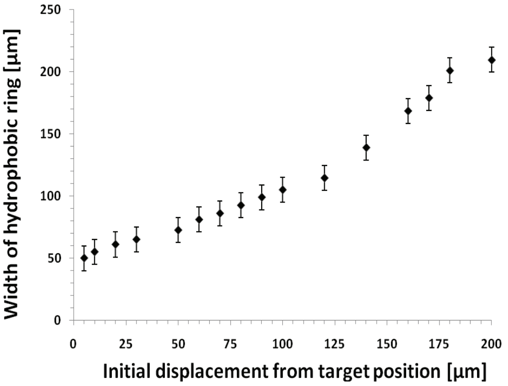

Figure 5: Width of the hydrophobic ring.

There is a non-linear behaviour which is caused by considering the deformation of the droplet shape and a damping by inner viscosity. As one can see in Figure 5 for the positioning of a droplet with an initial displacement of 50 µm the width of the hydrophobic ring must be about 70 µm.

5. Experimental Results

The necessary volume of the catching droplets for the fluidic-based assembly method is in the range of some nano-litres. The generation and deposition of catching droplets with a diameter of about 200 µm and a volume in the range of some nano-litres is very difficult. In the experiments regular dispensing systems and jet-type dispenser were used to generate the necessary small droplets with volumes in the range of nano-litres.

Figure 6 shows a catching droplet deposited by a regular dispensing system. The surface of the substrate is coated with PTFE and functionalized by a Laser to get the needed structure with well defined hydrophilic and hydrophobic domains.

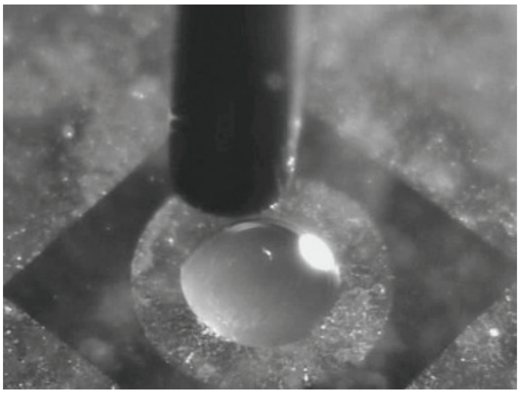

Figure 6: Positioning of a catching droplet with a regular dispenser.

The resulting structure has a very good lateral resolution with abrupt transitions from hydrophilic to hydrophobic areas. Here the droplet is deposited by delivering the fluid through a needle and contacting the surface by the fluid built up in the outlet of the needle. At the same time the needle is converged and diverged to the surface of the substrate. The resulting interface of the deposited droplet is built up through the surface tension of the fluid and the adhesion between the fluid and the surface. The droplet was dispensed with a well defined initial displacement of about 50 µm to its target position. In this experiment we observed a very fast self alignment of the catching droplet to its target area surrounded by the hydrophobic ring with a high accuracy.

The experimental deposition and positioning of a catching droplet by a jet-type dispenser is illustrated in Figure 7.

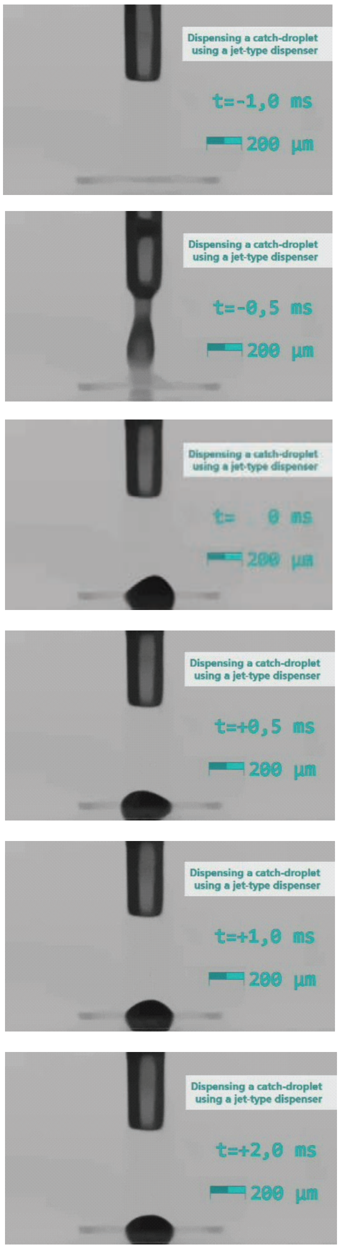

Figure 7: Positioning of a catching droplet with a jet-type dispenser.

The bouncing droplet has a diameter of about 200 µm and a volume of some nano-litres. It has a well defined initial displacement of about 50 µm from its final position (hydrophilic area) on the substrate.

After the droplet hits the substrate it accelerates in direction of the smaller contact angle (hydrophilic area) and a damped oscillation around the equilibrium state (final position) is resulting. This is the same qualitative behaviour as calculated by the numerical simulations (Figure 2). Here the oscillation frequency is about 1 kHz and therefore in about the same range as the simulation result (about 0.84 kHz). The time for positioning this droplet on the hydrophilic area (target position on substrate) from contacting the surface until a remaining displacement of less than 15 % to its final position is about 2 ms (see last picture in Figure 7). Comparing this result with the numerical calculated in Figure 4, where the time is about 2.7 ms for an initial displacement of 50 µm with a remaining displacement of 15 %, we observe a difference in time for positioning of about 0.7 ms. The cause of this difference between the experimental and the simulation results is a higher damping in the experiments. That means there is an additional or higher damping effect in the experiments which must be taken into account in the simulation model in future studies.

In general we can say the experimental result equals to the results calculated by numerical simulation. As a result of the experiments the catching droplet is positioned to a well defined area by use of a selective structured surface and different dispensing methods with a high accuracy. These studies were made to show the feasibility for positioning of a droplet to a well defined area by use of a structured surface as well as to achieve a qualitative verification of the simulation results.

7. Conclusions

The presented paper describes a novel fluidic-based selfassembly method. This method uses forces based on the predominant microfluidic effect caused by surface tension to move and position droplets.

The finite element method is used for modelling and simulation. The set of equations are solved by using "COMSOL Multiphysics" which allows also the coupling of different physical models and the simulation of multiphase problems [5].

Results of numerical simulations are presented and completed with experiments made in cooperation with the Fraunhofer IPA. The results show the capability for positioning of a droplet to a well defined area by use of structured surfaces. This is done within a short time which is in the range of some milliseconds.

Therefore this method for microassembly has potential to be a fast assembly process with a high throughput of assembled microchips (e.g. RFID or LED) per hour. In future the conventional assembly methods (e.g. die-bonder) for microchips could be extended by this fluidic-based method.

To show the feasibility and to develop this novel fluidic-based microassembly technology further studies of the dynamical behaviour of the droplet and the microchip have to be performed.

8. References

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