Simulation of the Self Assembly of a Microchip on a Structured Surface using the Phase Field Method

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Abstract: The presented paper describes a method for micro precision assembly of very small objects like future microchips, which have a lateral expansion equal to or smaller than 500 µm. The modelling and simulation of a fluidic-based micro assembly method for a microchip with a dimension of (500 x 500 x 100) µm³ is performed with COMSOL Multiphysics. The finite element method is used for modelling and simulation. The physical problem is modelled as a transient 2D Fluid-Structure Interaction (FSI) containing two separated fluid phases and a rigid body (microchip). The movement of the microchip is induced by the fluid and is described by the arbitrary Lagrangian-Eulerian (ALE) technique. The separated two-phase flow is modelled by using the Phase Field Method. Results from numerical analysis and simulations were evaluated.

Keywords: Phase Field Method, 2 Phase Fluid-Structure-Interaction, Micro Assembly, Self Assembly.

1. Introduction

The technological development towards miniaturization, higher integration as well as towards more cost efficiency makes it necessary to investigate a new assembly method for these micro components.
The presented assembly method is based on the use of small droplets and structured surfaces with hydrophilic and hydrophobic areas. As a driving force for assembly this fluidic-based technology uses surface tension which is predominant in the micro scale. The force is strong enough to move droplets to a well defined position (Berthier, *et al.*, 2006). With well defined hydrophilic and hydrophobic areas on the surface of a substrate it is possible to position droplets which move microchips to specified positions for assembly (Lambert, 2007).

2. Principle

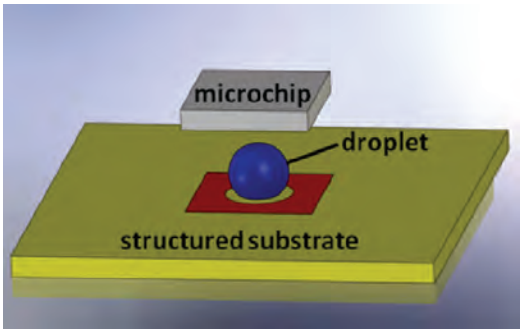

Figure 1. Principle of the fluidic self assembly of a microchip

As shown in figure 1 the process for selfassembly of a microchip is based on using a surface with hydrophilic and hydrophobic areas and a small portion of fluid (blue droplet) which is locally restricted to a well defined area on the substrate (Boufercha, *et al.*, 2009).
First the droplet with a diameter of 200 µm is placed to a well defined (hydrophilic) area where it is enclosed by a hydrophobic ring (orange ring in figure 1). After the deposition of the droplet on the substrate the microchip (green cuboid in figure 1) is deposited on top of the droplet. The wetting of the hydrophilic bottom side of the microchip by the droplet causes the droplet to override the hydrophobic ring. The final position for alignment of the microchip is marked by a rectangular boundary which forms a transition from a hydrophilic to a hydrophobic area. The movement is caused by the surface tension of the fluid and is a result of the minimization of the surface energy to achieve thermodynamic equilibrium.

3. COMSOL Multiphysics

The physical problem is given by the self assembly of a microchip on a structured substrate

by a droplet. It is modelled as a transient 2D Fluid-Structure Interaction (FSI) containing two separated fluid phases. The predefined Fluid-Structure Interaction application in the MEMS Module of COMSOL Multiphysics is used. The simulation illustrates how a fluid can induce movements on a rigid body (microchip) using the arbitrary Lagrangian-Eulerian (ALE) technique along with a separated two-phase flow using Phase Field application mode in the MEMS module.
The model geometry (see figure 2) consists of a rectangular domain, in which a rectangular rigid body (silicon microchip) is initially positioned on a well defined fluid portion (droplet). Initially the fluid of higher density (water) is present in the droplet sub domain and the fluid of lower density (air) is present everywhere else.

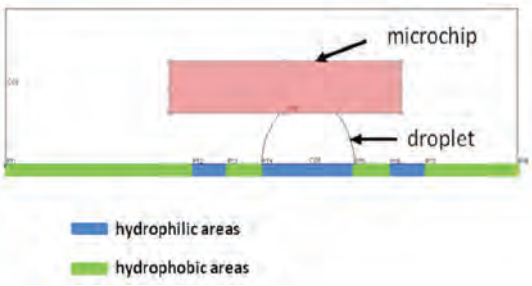

Figure 2. A schematic of the fluidic self assembly of a microchip

The dynamics of the moving geometry and the moving boundaries of the microchip are handled with a moving grid by the arbitrary Lagrangian-Eulerian (ALE) method. Both fluids have a very low Reynolds number and therefore a laminar flow is assumed. The moving interface between the two separated fluid phases (water droplet and air) is tracked using the phase field method. The surface of the microchip has a "moving wetted wall" boundary condition, which allows a contact angle and a wall velocity to be specified. This is resulting in a possible movement of the microchip. The new mesh coordinates of the moving mesh are computed based on the movement of the structure's (microchip) boundaries and the implemented default mesh smoothing of the predefined Fluid-Structure Interaction application.

In summary there is a coupling of three different physics:

1. Incompressible Navier-Stokes for both fluids (air and water),
2. a plane strain application for movement / deformation of the rigid body (silicon microchip)
3. and a Moving Mesh application for computing the deformation/movement of the finite elements mesh.

A transient analysis type and a time dependent solver are used for all three physics.

The computation is done by the following sequence:

1. Two-Phase Flow, Laminar, Phase Field application solves for the velocity, pressure and volume fraction of the two phases.
2. Plane Strain application mode solves the model's structural mechanics portion. The large deformation analysis is activated by default for more accurate computing of large strains. The solved deformation velocity (the velocity of the boundaries of the microchip) acts as the boundary condition for the Two-Phase Flow, Laminar, Phase Field and the Moving Mesh application modes.

Moving Mesh (ALE) application mode solves for the mesh deformation.

4. Equations and discretization scheme

The dynamical behaviour of the two immiscible fluids (air and water) is described by the Navier-Stokes-Equations (NSG) for incompressible fluids:

$$\rho\frac{\partial\vec{u}}{\partial t}+\rho\vec{u}\cdot\nabla\vec{u}-\nabla\cdot[-p\mathrm{I}+\eta(\nabla\vec{u}+\nabla\vec{u}^{T})]=F$$

$$\nabla\cdot\vec{\mathrm{u}}=0$$

ρ: density of fluid [kg/m³]
$\vec{u}$: velocity vector [m/s]
p: pressure [Pa]
η: dynamic viscosity [Pa·s]
F: volume force [N/m³]
I: dimensionless identity matrix

The dynamical behaviour of the interface between the two fluids is described by the Cahn-Hilliard-Equation:

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \nabla \cdot \gamma \nabla G$$

ϕ: dimensionless phase field variable
u: velocity [m/s]
γ: mobility [m³·s/kg]
G: chemical potential [N/m²]

The mobility γ is given by:

$$\gamma = \chi \cdot \varepsilon^2$$

ε: parameter controlling interface thickness [m]
χ: mobility tuning parameter [m·s/kg]

The chemical potential G is given by the relation:

$$G = \lambda \left[-\nabla^2 \phi + \frac{\phi(\phi^2 - 1)}{\varepsilon^2} \right]$$

λ: energy density [N]

The relationship between the energy density λ, the capillary thickness ε and the surface tension coefficient σ is given by the following equation:

$$\lambda = \frac{3\varepsilon\sigma}{2\sqrt{2}}$$

σ: surface tension coefficient [N/m]

For use in COMSOL Multiphysics the Cahn-Hilliard-Equation is separated into two coupled partial differential equations:

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \nabla \cdot \frac{\gamma \lambda}{\varepsilon^2} \nabla \psi$$

$$\psi = -\nabla \cdot \varepsilon^2 \nabla \phi + \left(\phi^2 - 1 \right) \cdot \phi + \left(\frac{\varepsilon^2}{\lambda} \right) \frac{\partial f_{ext}}{\partial \phi}$$

ψ: dimensionless variable
f_{ext}: external free energy [N/m²]

The set of coupled partial differential equations is solved by using the finite element method for spatial discretization (Zimmerman, 2006). The mesh is generated by use of the advancing front algorithm and individual element growth rates for each subdomain. Figure 3 shows the final criterions for the mesh element growth rates and sizes.

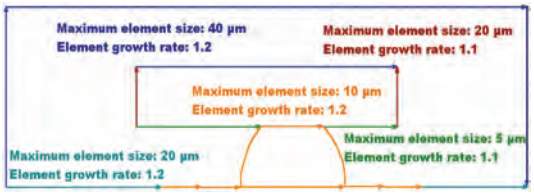

Figure 3. Growth rates and mesh element sizes

The resulting mesh is shown in the following figure 4. The base mesh exists of about 1600 mesh points and 3000 triangular elements. They are coloured according to their quality. The minimum element quality is 0.8514. The resulting extended mesh has about 30000 degrees of freedom.

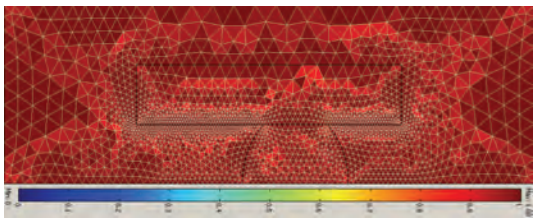

Figure 4. Mesh with coloured element quality

The time dependent equations are solved by use of a discretization in time with very small time step sizes. The initial time step size is 0.5 ns. Depending on the progress of the calculation it can be scaled up to 1 µs. This is usually possible after 10000 time steps. The total number of time steps for one calculation is about 20000.

5. Results

Figure 5 shows the simulation result of a silicon microchip (white) which is self aligned by a water droplet (red) on a structured surface with well defined wetting areas.

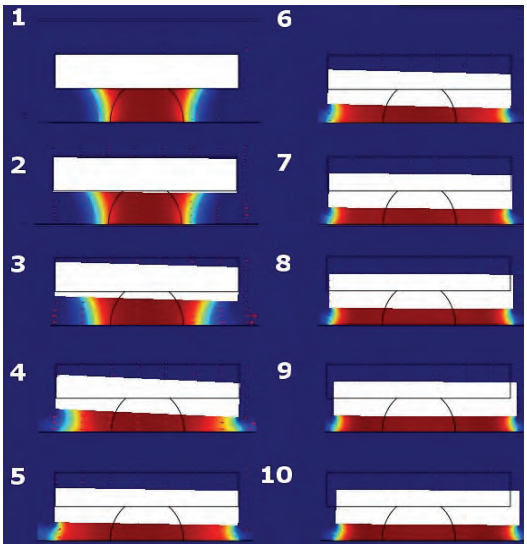

Figure 5. Simulation result for the self alignment of a silicon microchip

In this case the microchip has a small lateral initial displacement to its final position. The frames which are numbered from 1 to 10 show a temporal evolution of the transient simulation. The droplet which was restricted to a well defined area is moving outwards. The capillary force moves the fluid (red) outwards and pulls the microchip therefore (white) down until the water reaches the outer hydrophobic frontier. Then the movement is finished and the microchip has a stable position.

The total time for the displacement from position 1 to 10 in figure 3 is about 1 ms. That means that the microchip is placed fully on the target position and is ready for a further handling in about 1 ms.

Results from further simulations of the self alignment of a microchip for various lateral initial displacements of the microchip against its final assembly position showed a changing in time in the range of some milliseconds. The total time for a lateral initial displacement from 0 µm to 100 µm is in the range from 1 ms to 3 ms. As a result the microchip has an average velocity of up to 10 cm/s.

6. Conclusion

The presented paper describes a fluidic-based self assembly method for small objects like silicon microchips. This method uses forces based on the predominant micro fluidic effect, caused by surface tension. The set of equations are solved by using COMSOL Multiphysics which allows also the coupling of different physical models. The problem is studied by use of the predefined Fluid-Structure Interaction application in the MEMS Module of COMSOL Multiphysics. The results of numerical simulations show the capability of this fluidic-based selfassembly methods for aligning microchips with a dimension of (500 x 500 x 100) µm³. Additionally the total time for self alignment of a silicon microchip can be predicted. The order of magnitude of time for the fluidic-based selfassembly is also depending on the initial displacement of the microchip against its final assembly position. The total time for self alignment of a microchip without a lateral initial displacement is about 1 ms and the total time for a lateral initial displacement of up to 100 µm is in the range from 1 ms to 3 ms. The average velocity of the microchip is up to 10 cm/s.

7. References

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