Finite element simulation of solid-liquid phase transitions with a free melt surface

Alfred Schmidt

(joint work with Eberhard Bänsch, Thilo Moshagen, and Jordi Paul)

Introduction. The Collaborative Research Centre 747 "Micro cold forming" studies aspects of the production of micro components. Motivated by the engineering application of melting the end of thin wires by laser heating in order to accumulate material for a subsequent forming process, we study the melting and solidification of material with a free capillary melt surface. The model leads to a coupled system of Stefan and Navier-Stokes equations, where the solution of the Stefan problem defines the solid subdomain $\Omega_s(t)$ and the solution of Navier-Stokes with capillary boundary gives the shape of the liquid subdomain $\Omega_l(t)$. An Arbitrary Lagrangian Eulerian Finite Element method is presented that is able to compute a numerical solution without spurious oscillations.

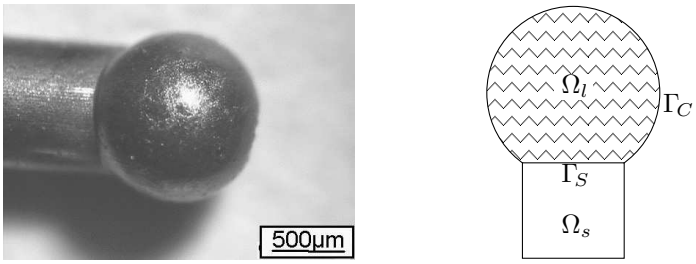

Figure 1. Left: material accumulation from experiment; right: solid and liquid subdomains Ω_s and Ω_l, interface Γ_S and capillary surface Γ_C.

Mathematical Model. The nondimensional system of equations for temperature θ, pressure p, velocity field u and time-dependent domain $\Omega(t) = \Omega_s(t) \cup \Omega_l(t) \cup \Gamma_S(t)$ (see Figure 1) consists of a Stefan problem for the temperature,

$$\frac{\partial}{\partial t}\theta + u \cdot \nabla\theta - \frac{1}{Re\,Pr}\Delta\theta = 0 \text{ in } \Omega_l(t), \quad \frac{\partial}{\partial t}\theta - \frac{1}{Re\,Pr}\frac{\kappa_s}{\kappa_l}\Delta\theta = 0 \text{ in } \Omega_s(t),$$

with Stefan boundary conditions on the solid-liquid interface $\Gamma_S(t) = \bar{\Omega}_l(t) \cap \bar{\Omega}_s(t)$

$$\theta = 0, \quad \frac{St}{Re\,Pr}\Big[\partial_\nu\theta_{|\Omega_l} - \frac{\kappa_s}{\kappa_l}\partial_\nu\theta_{|\Omega_s}\Big] = V_{\Gamma_S} \quad \text{on } \Gamma_S(t)$$

and heat flux condition including laser heating and radiation on the outer boundary

$$\partial_\nu\theta = La\, I_l + Em(\theta_a^4 - (\theta_m + \theta)^4) \quad \text{on } \partial\Omega(t),$$

coupled with Navier-Stokes equations in the liquid subdomain $\Omega_l(t)$

$$\frac{\partial}{\partial t}u + u \cdot \nabla u - \nabla \cdot \left(\frac{1}{Re}\mathbf{D}(u) - p\,I\right) = -\frac{Bo}{We}e_z + \frac{Gr}{Re^2}\theta\, e_z, \quad \nabla \cdot u = 0$$

with no-slip condition $u = 0$ on the solid-liquid interface $\Gamma_S(t)$ and capillary condition on the free melt surface $\Gamma_C(t) = \partial\Omega_l(t) \setminus \Gamma_S(t)$

$$u \cdot \nu = V_{\Gamma_C}, \quad \sigma\nu = \frac{1}{We}\mathcal{H}\nu, \quad \text{on } \Gamma_C(t).$$

Here, Re, Pr, Bo, We, Gr, and St denote the Reynolds, Prandtl, Bond, Weber, Grasshoff, and Stefan numbers, La and Em the laser power and emissivity constants, I_l is the intensity distribution of the laser heating, $\mathcal{H}$ the mean curvature of the capillary boundary.

Finite element methods. The finite element discretization of this system can be done separately for the Stefan problem in an enthalpy formulation as studied in [3] and for the Navier-Stokes system as in [1]. For an application *without* capillary boundary (Bridgman growth of a semiconducter crystal), the coupled numerical method was demonstrated sucessfully in [2]. There, on a fixed mesh, the discrete liquid subdomain is given by all mesh elements, where the temperature is above melting temperature (nondimensional, $\theta > 0$).

When the capillary boundary meets the phase boundary in a triple line (or point in 2D), a coupled method of the type mentioned above is possible, too, but can easily produce spurious velocity oscillations. This is due to the fact that whole mesh elements change from solid to liquid and thus parts of the outer boundary change from solid to capillary boundary. The capillary forces directly push the boundary element into a different position, which produces a strong local velocity. Thus, a new approach had to be developed.

The new method presented here uses a representation of the phase boundary by mesh lines (in 2D, faces in 3D) and a front tracking method. Using the strong formulation of the Stefan problem, the velocity of the phase boundary can be computed from the jump of temperature gradients. Moving local mesh points by the velocity of the interface (which is a non-material velocity), we end up in an *Arbitrary Lagrangian Eulerian* (ALE) formulation of the coupled system. A similar approach is used for moving the mesh with the capillary surface. Special attention must be directed to the triple junction where capillary surface and solid-liquid interface meet.

As the moving mesh degenerates when the liquid subdomain changes much, as in our application, remeshing is necessary at certain times. In order to not reduce the resolution of free boundaries, we keep the mesh points on the capillary boundary and interface and generate a new mesh only for the interior of the solid and liquid subdomains.

Numerical results. Both a 2D and a 2D axial symmetric implementation of the algorithm were done based on the Navier code [1], the remeshing is done using by Triangle [5]. Figure 2 shows a zoom into the mesh around the solid-liquid interface at two different times from a 2D axial symmetric simulation. The interface lies in the light gray region. Mesh lines at the interface were moved together with it, and the bulk was remeshed between the two time instances.

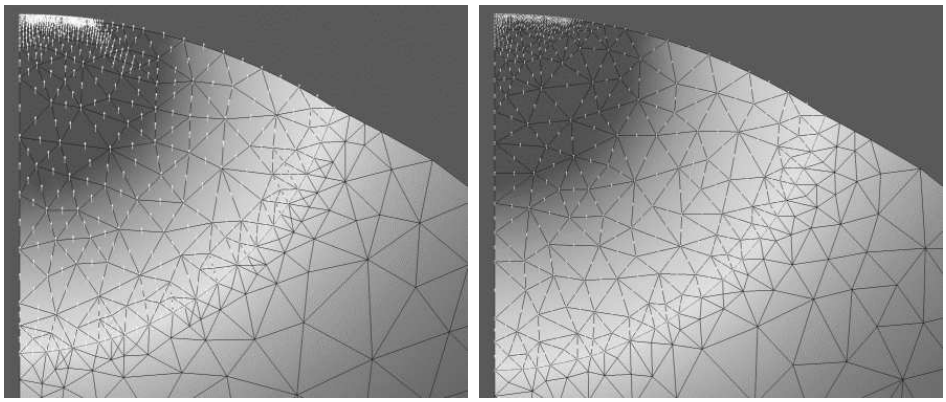

FIGURE 2. Meshes from two different time steps. Gray shade indicates temperature, the interface lies in the light region.

Work in progress. As the front tracking approach is applicable only when already some liquid pool exists, a combination with the enthalpy formulation FEM is needed in the beginning of the process, until some material is molten.

Some open questions and related future work regard the optimization of microstructure in the re-solidified material by a time-dependent control of laser power.

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E. Bänsch and J. Paul: AM3, Department Mathematik, Universität Erlangen-Nürnberg,

T. Moshagen and A. Schmidt: Zentrum für Technomathematik, FB 3, Universität Bremen.