MODELING OF MELTING AND SOLIDIFICATION PROCESSES OF PHOTOVOLTAIC SILICON IN A TRAVELING MAGNETIC FIELD

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Abstract: Directional solidification of silicon is modeled using a gallium volume with a square horizontal cross-section and dimensions of 10x10x7.5 cm^3. The container with gallium is heated at the top and cooled at the bottom. It is placed in a coil system generating a traveling magnetic field. Coupled 3D numerical simulations of melt flow and phase interface are carried out and compared to first experimental measurements of temperatures in gallium and the phase interface motion. The transfer of the results to silicon melts using scaling laws is discussed.

1. Introduction

The directional solidification process is used in the photovoltaic industry to produce large silicon ingots with a weight up to 1000 kg. In a crystallization furnace, silicon raw material is first melted and then directionally solidified in a square-shaped silica crucible that is surrounded by several heaters at the side or top and a heat sink at the bottom. In the liquid silicon, a flow is usually generated by buoyancy or Marangoni forces as well as by Lorentz forces due to alternating currents in the heaters or additional inductors. It has been shown that there is a tight mutual interaction between the melt flow and the shape and velocity of the melting or solidification interface [1]. Melt flow may significantly change the temperature gradients and the phase interface shape, whereas a geometrically large deformation of the interface may lead to significant changes in the flow pattern. For example, the effect of small Lorentz force inhomogeneities on the flow pattern can be considerably increased due to this interaction [1].

Direct experimental investigations of processes in silicon melts are generally very complicated due to the high melting point of 1685 K. While numerical simulations can be a very useful tool for such investigations, the numerical models must be verified and validated. This can be achieved using model experiments in low-melting-point low-Prandtl-number metals, such as gallium. Pure gallium allows for an induction of Lorentz forces similarly to a silicon melt and can be also solidified in a controlled manner [2, 3, 4].

A new experimental setup for model experiments has been developed recently [5]. It contains a model melt with a square horizontal cross-section of 10x10 cm^2 and variable height up to 10 cm. The melt is located within a coil system that generates a traveling magnetic field (TMF). A cooling system at the bottom and a heating system at the top of the melt enable to generate a vertical temperature difference up to about 50 K. Various experiments with a GaInSn melt and ultrasonic measurements of the flow pattern as well as temperature measurements with thermocouples have been already presented in [5]. This contribution focuses on melting and solidification processes of gallium in this experimental setup. Thermal regimes of the heater

and cooler to obtain a continuous phase interface movement are discussed. The coupled problem of melt flow and phase interface motion under the influence of a magnetic field is investigated by 3D numerical simulations.

2. Numerical model

The 3D time-averaged Lorentz force F_L induced by the TMF in the melt was calculated using the finite element package *GetDP* by solving the time-harmonic equations for the electric and magnetic potentials V and A:

$$\nabla\times\nabla\times\vec{A}=\mu_0\vec{j}\,,\quad \nabla\cdot\vec{j}=0\,,\quad \vec{B}=\nabla\times\vec{A}\,,\quad \vec{j}=\sigma\left(-i\omega\vec{A}-\nabla V\right),\quad \vec{F}_L=\left(\vec{j}^{\,*}\times\vec{B}\right)_{re}/2\,,$$

where j is the current density, B is the magnetic field, and $\omega=2\pi f$ is the current frequency. Material properties are given in Tab. 1. See [6] for further details. The Lorentz force was imported into the finite volume package *OpenFOAM*, which was used to solve the coupled unsteady equations of melt velocity u and melt/ crystal temperature T:

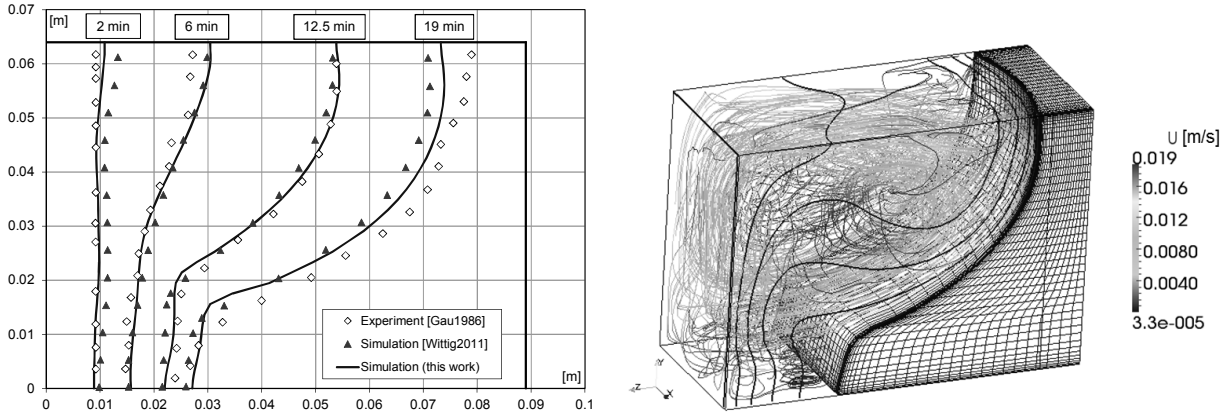
$$\rho\left[\frac{\partial\vec{u}}{\partial t}+(\vec{u}\cdot\nabla)\vec{u}\right]=-\nabla p+\eta\Delta\vec{u}+\vec{F}_L-\beta(T-T_0)\rho\vec{g}\,,\quad \nabla\cdot\vec{u}=0\,,\quad \rho c\left[\frac{\partial T}{\partial t}+(\vec{u}\cdot\nabla)T\right]=\lambda\Delta T$$

In each time step, the finite volume grid was deformed according to the interface velocity distribution v_n, which was calculated from the local heat balance on the solid (S) and liquid (L) sides: $v_n\rho_S q_0=\lambda_S\partial T/\partial n\big|_S-\lambda_L\partial T/\partial n\big|_L$. See [1] for further details of the model.

Property	**Symbol, Units**	**Ga: solid**	**Ga: liquid**	**Si: solid**	**Si: liquid**
Density	ρ [kg/m^3]	5904	6116	2329	2520
Viscosity	η [Pa·s]	-	0.00213	-	0.00076
Specific heat	c [J/kg·K]	374	360	986	986
Therm. conductivity	λ [W/m·K]	40.8	34.1	22	67
Therm. expansion	β [1/K]	-	0.00013	-	0.000144
Elec. conductivity	σ [S/m]	-	3.9e6	-	1e6
Latent heat	q_0 [J/kg]	8e4 (29.76 °C)	-	1.8e6 (1412 °C)	-

Table 1: Material properties of solid and liquid gallium (e.g., [7]) and silicon [1] used in this study.

The model was tested with a benchmark [2] for the melting of gallium influenced by buoyancy forces. An initially solid volume of 64x38x89 mm^3 is considered with a prescribed temperature T_H = 38 °C on the left and T_C = 28.3 °C on the right wall. Melting starts at the left (hot) wall, with the interface moving toward the right wall. A 3D simulation was carried out with 30x43x33 fluid and 30x43x27 solid elements, with the initial melt grid compressed to 4.5 mm (this introduces a time offset of about 1 min). The interface shape for several time instants is shown in Fig. 1 and demonstrates a good agreement with both experimental and numerical literature data.



(a) (b)

Figure 1: (a) Calculated melting interface shape for several time instants in comparison with literature data [2, 8]; (b) Deformed crystal mesh, flow streamlines, and temperature isolines at the walls in the simulation after 20 min.

3. Numerical results

We consider the experimental setup from [5] but with pure gallium instead of GaInSn, with a height of 7.5 cm. The Lorentz force distribution (see Fig. 2) from [5] for GaInSn with a height of 5 cm is used here for gallium neglecting the relatively small difference in electrical conductivities. Furthermore, the force distribution is deformed in *OpenFOAM* together with the grid, without recalculation for different melt heights. The grid in *OpenFOAM* consists of 42x42x27 fluid elements and 42x42x13 solid elements, the melt height is initially compressed to 3.8 mm. No slip conditions on all melt boundaries are used for the velocity field; buoyancy and Lorentz forces are considered in the volume. Sidewalls are assumed adiabatic for the temperature calculation. At the crystal bottom and melt top, heat transfer between gallium and heater (H) or cooler (C) is described according to $\lambda_{S/L}\partial T/\partial n\big|_{S/L} = p_{C/H}(T - T_{C/H})$. The heat transfer coefficient $p_{C/H}$ = 1563 W/m^{2}K from [5] is applied.

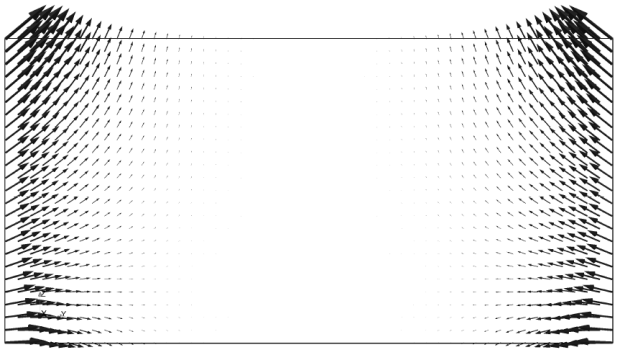
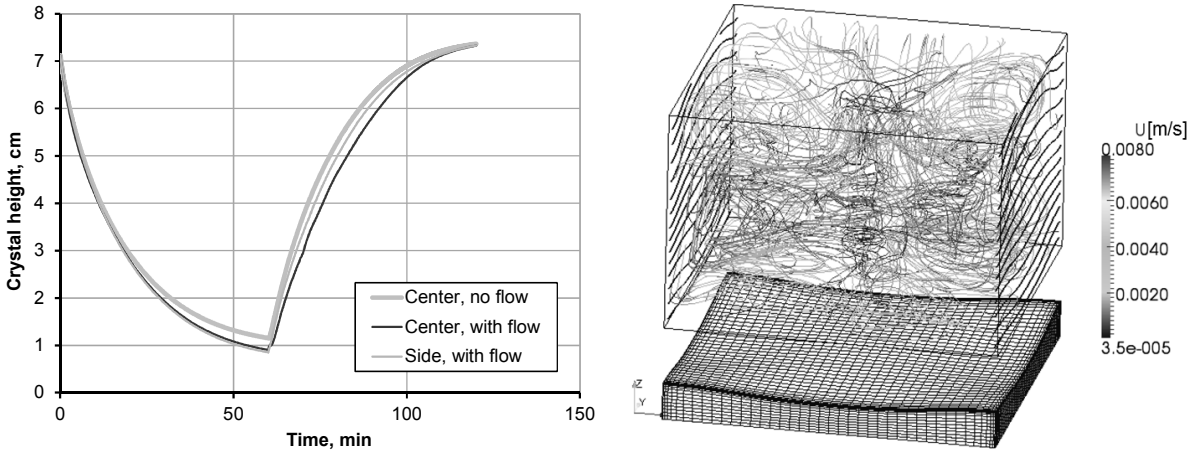


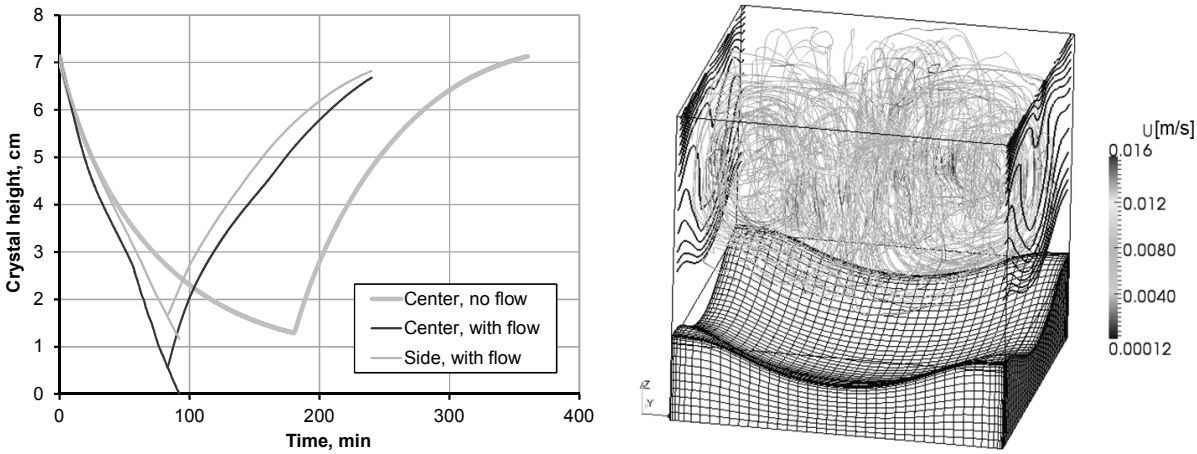
Figure 2: Lorentz force distribution in a vertical cut (F_{Lmax} = 115 N/m^3) for a melt height of 5 cm due to 6 coils generating an upward TMF with a frequency of 50 Hz [5].

Two simulations were carried out with different vertical temperature gradients (approximately 1 K/cm and 4 K/cm in the melt without flow), which were set by the cooler/ heater temperatures T_C/ T_H. Solid gallium is first melted down to approximately 1 cm thickness in the center, then the cooler/ heater temperatures are switched and the melt is solidified again. The results are summarized in Fig. 3. It can be seen that a 4 times higher temperature gradient

leads to about 3 times shorter melting and solidification times in the cases without melt flow. The melt flow reaches only 8 mm/s with a high (stabilizing) temperature gradient and has practically no influence on the phase interface, see Fig. 3(a). A low temperature gradient is not able to damp the TMF-induced flow structure, the melting time is significantly reduced due to the flow, and the phase interface develops a deflection of about 1 cm.



(a) Melting: T_H / T_C = 64.5/ 17.8 °C; solidification: T_H / T_C = 38.5/ −3.9 °C



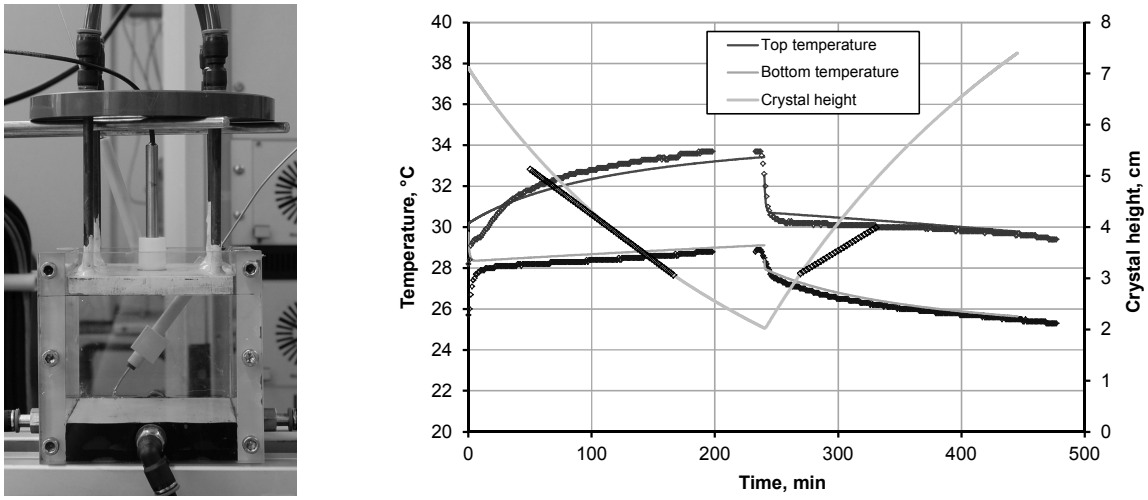
(b) Melting: T_H / T_C = 38.5/ 26.8 °C; solidification: T_H / T_C = 32.0/ 21.4 °C

Figure 3: Numerical simulations with various heater/ cooler temperatures (a,b). Phase interface motion in the center and at the side (left); deformed crystal mesh, flow streamlines, and temperature isolines at the walls after the melting phase (right).

4. Experimental results

The experimental setup as described in the previous section and in [5] was adjusted for experiments with gallium. A slightly different cooler design, stronger joints between the sidewalls, new coatings of the heater and cooler were introduced in particular. The most important changes for numerical modeling are different heat transfer coefficients of the heater (temperature T_H) and cooler (temperature T_C). They were determined from measurements of temperatures at the top (T_T) and bottom (T_B) of solid or liquid gallium of height H. With an approximate vertical heat flux density through gallium $q = \lambda_{S/L}\left(T_T - T_B\right)/H$ it was estimated $p_C = q/\left|T_C - T_B\right| = 600$ and $p_H = q/\left|T_H - T_T\right| = 450$ W/m^{2}K.

Fig. 4 summarizes the first experimental results. Solid gallium of 7.5 cm height was first melted and then solidified without TMF. In addition to the temperatures at the top and bottom, phase interface motion was measured by ultrasonic Doppler velocimetry through the heater using the equipment from [5]. While the temperatures and the melting rate agree well with numerical calculations, the solidification rate shows some deviations. These might be caused by an asymmetric phase interface, probably due to the anisotropic thermal conductivity of solid gallium [2]. Further experiments are required to evaluate the reproducibility of these results.



(a) (b)

Figure 4: (a) Photo of the experimental setup (without melt); (b) measured (dots) and calculated (lines) temperatures and interface position during melting (T_H / T_C = 38.5/ 26.8 °C) and solidification (T_H / T_C = 32.0/ 21.4 °C) without TMF.

5. Scaling of results

The topic of scaling between small-scale model experiments with GaInSn and silicon processes has been discussed in [5, 6]. The same approach can be used also for gallium, with additional parameters describing the phase change. We consider scaling from gallium (the case with solidification in Fig. 3(b)) with a characteristic length L_0 = 5 cm to silicon with L_0 = 10 cm. The following dimensionless numbers can be kept constant

$$S_{EM} = \mu_0 \sigma \omega L_0^2 = 3.8\,,\ F_{EM} = F_{L0}\frac{L_0^3 \rho_L}{\eta^2} = 2\cdot 10^7\,,\ J_{S/L} = \lambda_{S/L}\frac{\Delta T_{S/L}}{q_0 \rho_S L_0 v_0} = 2.5/0.5$$

by adjusting the frequency f = 50 → 48 Hz, Lorentz force density (by inductor current) F_{L0} = 115 → 4.5 N/m^3, temperature difference in the melt ΔT_L = 2 → 5 K and crystal ΔT_S = 8 → 68 K. As a consequence the flow velocity changes as u_0 = 1 → 0.4 cm/s and solidification velocity as v_0 = 2 → 0.5 cm/h. The Peclet and Grashof numbers are not kept constant:

$$Re = \frac{u_0 L_0 \rho_L}{\eta} = 10^3\,,\ Pe_V = \frac{\rho_S c_S L_0 v_0}{\lambda_S} = 0.015\,,\ Pe = \frac{\rho_L c_L L_0 u_0}{\lambda_L} = \begin{cases} 32\,(\mathrm{Ga}) \\ 16\,(\mathrm{Si}) \end{cases},$$

$$Gr = \frac{\rho_L^2 g \beta \Delta T_L L_0^3}{\eta^2} = \begin{cases} 3\cdot 10^6\,(\mathrm{Ga}) \\ 8\cdot 10^7\,(\mathrm{Si}) \end{cases}$$

Consequently, only phase change and melt flow with Lorentz forces dominating over buoyancy forces ($Gr << F_{EM}$) can be transferred to a larger silicon melt with the current scaling scheme.

6. Conclusions

Numerical simulations of the melting and solidification of gallium show that a TMF-induced flow can increase the melting rate several times but also leads to a deflected phase interface. A high stabilizing temperature gradient damps the TMF flow and reduces the role of the melt flow. First melting and solidification experiments of gallium without TMF were successfully carried out.

Acknowledgment

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