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Modeling of Silicon Transport into Germanium Using a Simplified Crystal Growth Technique

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Abstract

- **A numerical simulation study, using COMSOL Multiphysics, was carried out to examine the temperature and concentration fields in the dissolution process of silicon into germanium melt. This work utilized a simplified configuration which may be considered to be similar material configuration to that used in the Vertical Bridgman growth methods. The concentration profile for the SiGe sample processed using this technique shows increasing transport silicon into the melt with time, moreover, a flat stable interface is observed. The mass and momentum equations for fluid flow, the energy and the solute mass transport were numerically solved using COMSOL package. Results showed good agreements with experiments.**

Mathematical Model and Modeling Using COMSOL

Governing Equations for liquid phase

$$\nabla \cdot \vec{V} = 0 \qquad (1)$$

$$\rho_L \frac{\partial \vec{V}}{\partial t} + \rho_L \vec{V} \nabla \cdot \vec{V} = -\nabla p + \mu_L \nabla^2 \vec{V} + \rho \vec{g} \qquad (2)$$

$$\rho_L cp_L \frac{\partial T}{\partial t} + \rho_L cp_L \vec{V} \nabla \cdot T = k_L \nabla^2 T \qquad (3)$$

$$\frac{\partial C}{\partial t} + \vec{V} \nabla \cdot C = D_L \nabla^2 C \qquad (4)$$

Solid phase

$$\frac{\partial T_s}{\partial t} = \frac{k_S}{\rho_s cp_s} \nabla^2 T_s$$

Interface condition

At the dissolution interface we have saturation concentration defined as (in molar concentration silicon):

$$1 - \left(\begin{array}{l} 1.05513 \times 10^{-8} T^3 - 3.446005 \times 10^{-5} T^2 \\ + 0.038741\, T - 14.749675 \end{array} \right)$$

Numerical Resolution

COMSOL Multiphysics is able to solve complex multiphysics coupling in complex geometry. For instance, Navier-Stokes equations, energy and species conservations equations for example see references [19, 20]. The present simulation for the convective flow field, driven by both thermal/solutal buoyancy forces, is carried out by means of COMSOL Multiphysics package.

In the resolution procedure, the mesh choice should only be viewed as a compromise between convergence and solver memory requirement.

A coarser mesh with 19095 elements and a finer mesh with 23280 elements are considered. Results obtained, using the coarser mesh, are compared with those obtained using the finer mesh, the relative difference was found negligible (less than 3%). Therefore, all calculations carried out in this work are based using the finer mesh.

Results and Discussions

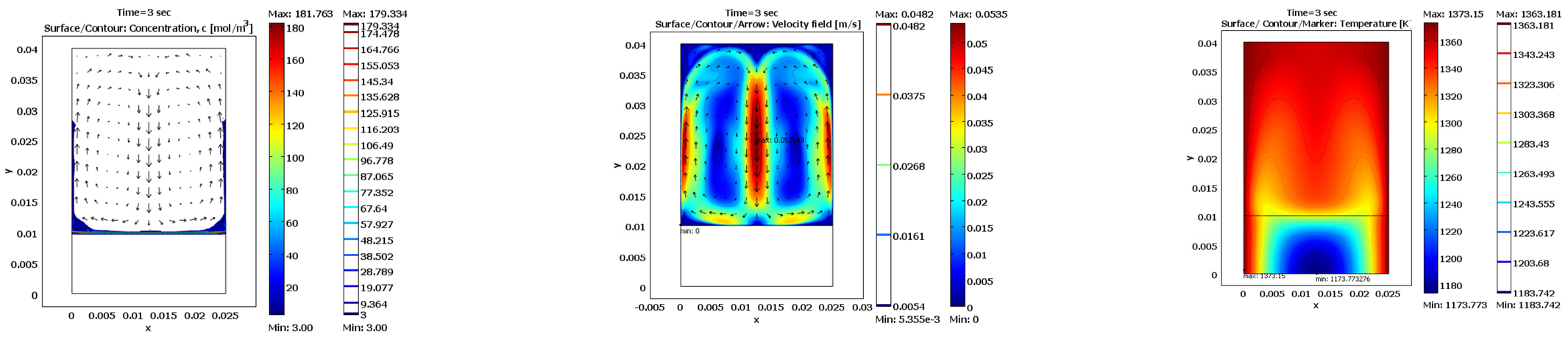

Fig. 1: Results after 3 secondes

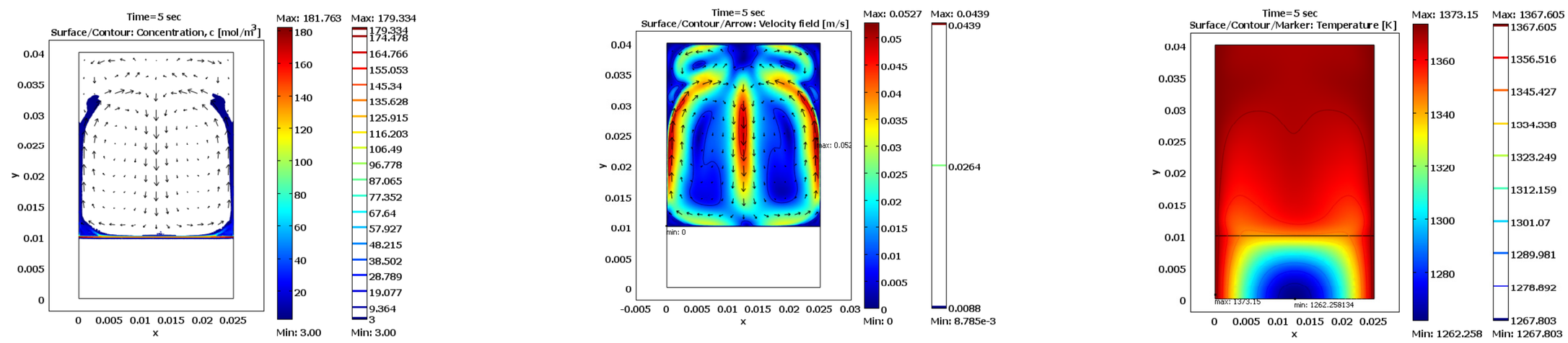

Fig. 2: Results after 5 secondes

Concentration, Convection-dominated flow and Temperature fields

-The simulation exhibited decomposing dissolution phenomena and showed an expected convection-dominated behavior. Examination for figure 2a and 3b shows a fit increasing dissolution rate.

-Thermo-solutal convection contributes to the dissolution phenomena for the present configuration (which may be considered as a simplified 2D Bridgman crystal growth case). This contribution was experimentally verified. In fact, like in experimental work by Dost and Coworkers [12] performed on the LPD (Liquid Phase Diffusion) process; the silicon dissolves from the bottom of the melt. Experiment was reported, that dissolution takes, experiments [12], just over 10 min to dissolve 2 mm of silicon. This indicates the strong effect of gravity on the dissolution mechanism. This is due to the fact that for the high-density difference between Silicon and Germanium. Silicon is substantially less dense than germanium and is therefore buoyant in the melt. With the dissolution interface at the bottom, the buoyancy of the silicon contributes to its transport upwards into the melt. This phenomenon increases the contribution of convective flow and causes the transport to become convection dominated.

Conclusions

A numerical simulation study, using COMSOL Multiphysics, was carried out to examine the velocity, temperature and concentration fields in the dissolution process of silicon into germanium melt. We use a simplified 2-D configuration which may be considered to be similar material configuration to that used in the Vertical Bridgman growth method. The concentration profile for the SiGe sample processed using this technique shows increasing transport silicon into the melt with time.

The strong effect of gravity on dissolution phenomena is illustrated. With the dissolution interface at the bottom, the buoyancy of the silicon contributes to its transport upwards into the melt. This phenomenon increases the contribution of convective flow and causes the transport to become convection dominated. This was tested experimentally.

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