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.

Keywords: COMSOL, Semiconductor, Crystal growth techniques, dissolution.

1. Introduction

Processing raw materials from the melt is the most important production principle for a large range of material classes [1]. Melt-grown single crystals of semiconductor materials are extremely valuable to the electronic industry, as they are the building blocks for the integrated circuit technologies. Thus, wafers cut from such crystals require having consistently uniform electrical properties to ensure a higher reproducibility and yield of solid-state devices. Consequently, there is enormous economic motivation to produce completely homogeneous crystals.

Generally bulk single crystals like semiconductors are grown either by crystal pulling (Czochralski method), vertical gradient freezing (Bridgman method) [2], Float Zone method [3] or Axial Heat Processing (AHP) technique [4] etc... All these processes have in common, that the growth process is influenced by a large number of process parameters.

Controlling these parameters means improving the final product. What makes the situation complex is the fact that during growth typically processes on different length scales are involved, [5, 6]. Maybe the most significant obstacle to achieving homogeneous crystals at faster growth rates is the phenomenon of morphological instability. This phenomenon is characterized by a sudden change in the shape of the solid/liquid interface during growth. This causes severe solute segregation and the destruction of crystal perfection via the formation of defects [4, 7, 8-10]. The result is a crystal with an undesirable variation in electrical properties that is unsuitable for electronic component production. Process parameters known to affect the stability of an interface include solid and liquid temperature gradients, the solidification or pulling rate, concentration of the solute, and melt flow [2, 4, 11].

The present study is devoted to investigating the influence of growth conditions on the dissolution process in Si-Ge system using a simplified crystal growth technique. The Si-Ge system was chosen due to its potentially greater application in electronic industry [11-14].

2. General Considerations and Mathematical Background

A schematic for the mold configuration used in this work is shown on figure 1. It consists of a cavity, of height H and length L, for simplification; in the present study we take a bi-dimensional case. The geometry chosen may be considered as a simplified vertical Bridgman configuration. It filled with a solvent Germanium melt, and a solute Silicon, which was taken at the bottom of the mold. The both mold right and the left walls were kept at a high temperature, T_{hot}.

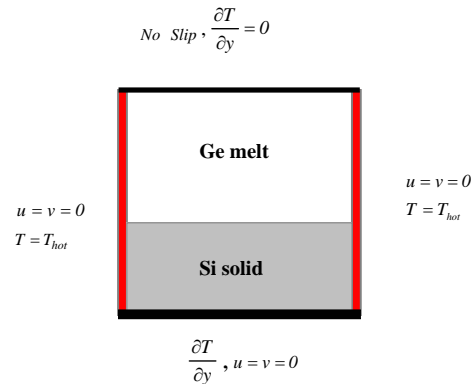The upper wall and the lower wall are considered to be adiabatic (Fig.1).

Governing Equations for liquid phase

Assumptions regarding the nature of the fluid in the present system may be summarized as: only laminar flow and Newtonian, incompressible, are considered, no internal heat generation or absorption are considered. No-slip velocity conditions on all boundaries. Thus, the governing equations, [15-17], that describe fluid motion and interfacial transport are:

Continuity
$$\nabla \cdot \vec{V} = 0 \qquad (1)$$
where $\vec{V}$ is the mass average velocity of the fluid (melt).

$$No\ Slip, \frac{\partial T}{\partial y} = 0$$

Ge melt

$u = v = 0$
$T = T_{hot}$

$u = v = 0$
$T = T_{hot}$

Si solid

$$\frac{\partial T}{\partial y}, u = v = 0$$

Figure 1. Schematic for Bridgman configuration and boundary conditions

Momentum transport

In most buoyancy-driven convection problems, convective flow is generated by both temperature and concentration variations in the fluid system, and which are difficult to avoid during crystal growth. These gradients lead to local density differences. To account for these effects, one method of consideration frequently used is the Boussinesq approximation, which, considers that the density of the fluid is assumed to be constant everywhere in the governing equations except in front of the gravity vector.. Thus the momentum balance (Navier-Stokes equation) may be expressed as:

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

where p and μ_L are the pressure, and viscosity of the fluid, respectively, and $\vec{g}$ is the gravitational vector.

Energy transport

Assuming no heat transfer by radiation, the thermal energy balance equation for the present work is given by

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

where K_L is the thermal conductivity of the fluid.

Solute transport

Assuming no diffusion in the solid, the solute transport equation is given by:

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

Solid phase

The problem can be greatly simplified assuming that there is no species diffusion in the solid so that $\vec{V} = 0$. The only additional equation needed is then

$$\frac{\partial T_s}{\partial t} = \frac{k_S}{\rho_s cp_s} \nabla^2 T_s \qquad (3)$$

where K_s is the thermal conductivity of the solid.

The thermo-physical properties of the Si-Ge system are given in [12-14].

Interface condition

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

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

2. Numerical resolution by COMSOL

COMSOL Multiphysics [18] 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)

(b)

(c)
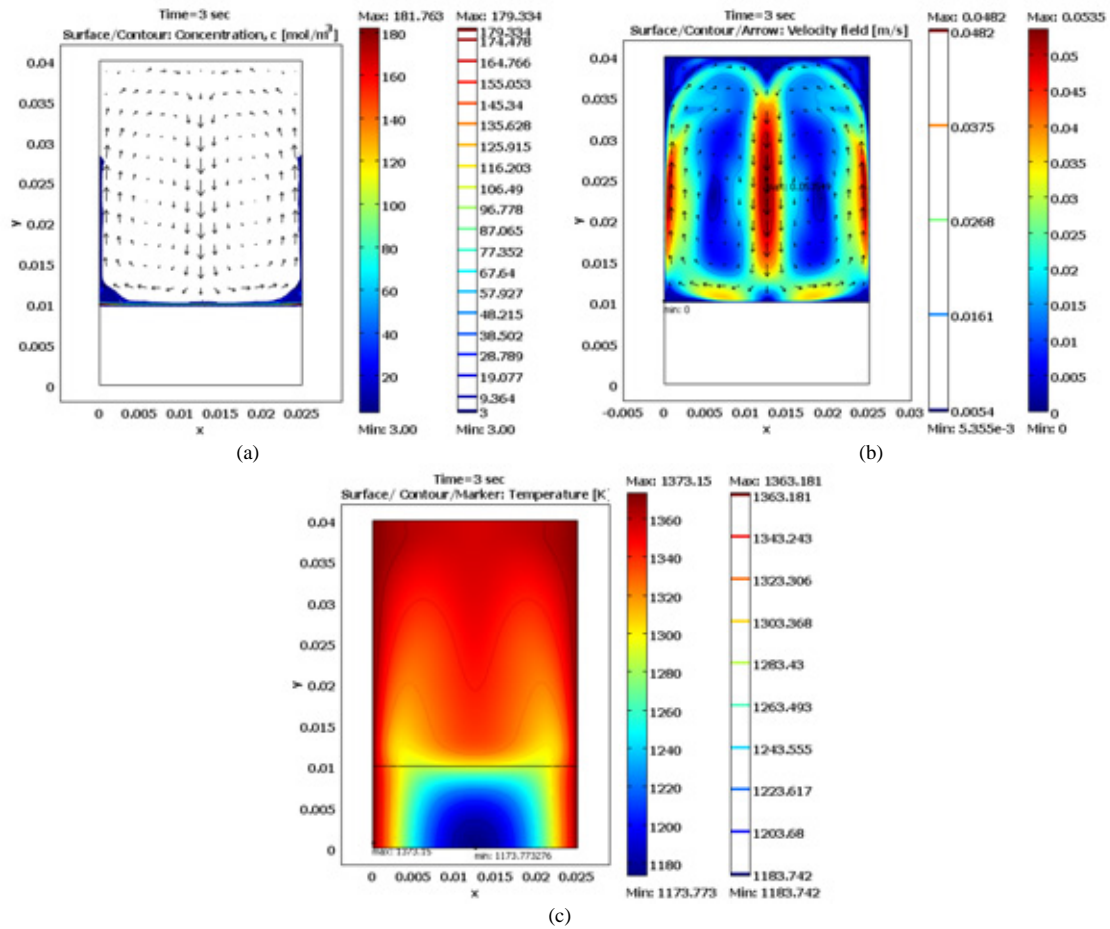
Figure 2. Results obtained after 3 seconds

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.

3. Results and discussion

COMSOL numerical results are presented, in order to demonstrate buoyancy-driven convection effects.

Concentration, Convection-dominated flow and Temperature fields

The simulations conducted for the present configuration, exhibited decomposing dissolution phenomena and showed an expected

convection-dominated behavior. The time evolution of the dissolution showed this decomposition increase trend. For instance, after 3 and 5 seconds concentration fields are presented in Figs. 2a and 3a, respectively. Examination for figure 2a and 3b shows a fit increasing dissolution rate.

Figure 3b shows that and instability is presented in the melt. In fact the flow bifurcates and begins asymmetric with respect of symmetric plane (y-axis). This is coherent because it is well known that when the thermal and solutal Rayleigh numbers, Ra_T and Ra_C, which give an indication of the level of convection in a system; and they are defined as thermal/solutal buoyancy force divided by viscous force, respectively. If the values of either Ra_T or Ra_C exceed a critical value, then convective instabilities (multiple convective cells/rolls) are predicted. For instance see

reference [21]. For the present configuration characterized by too large thermal and solutal Rayleigh numbers ($Ra_T = 3.8 \times 10^5$, $Ra_C = 8 \times 10^5$), too large to critical values for bifurcation. Thus, 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.

For the thermal field, since, the simulations were conducted under isothermal conditions; therefore, temperature gradients were minimized with time see Figs. 2c and 3c.

5. 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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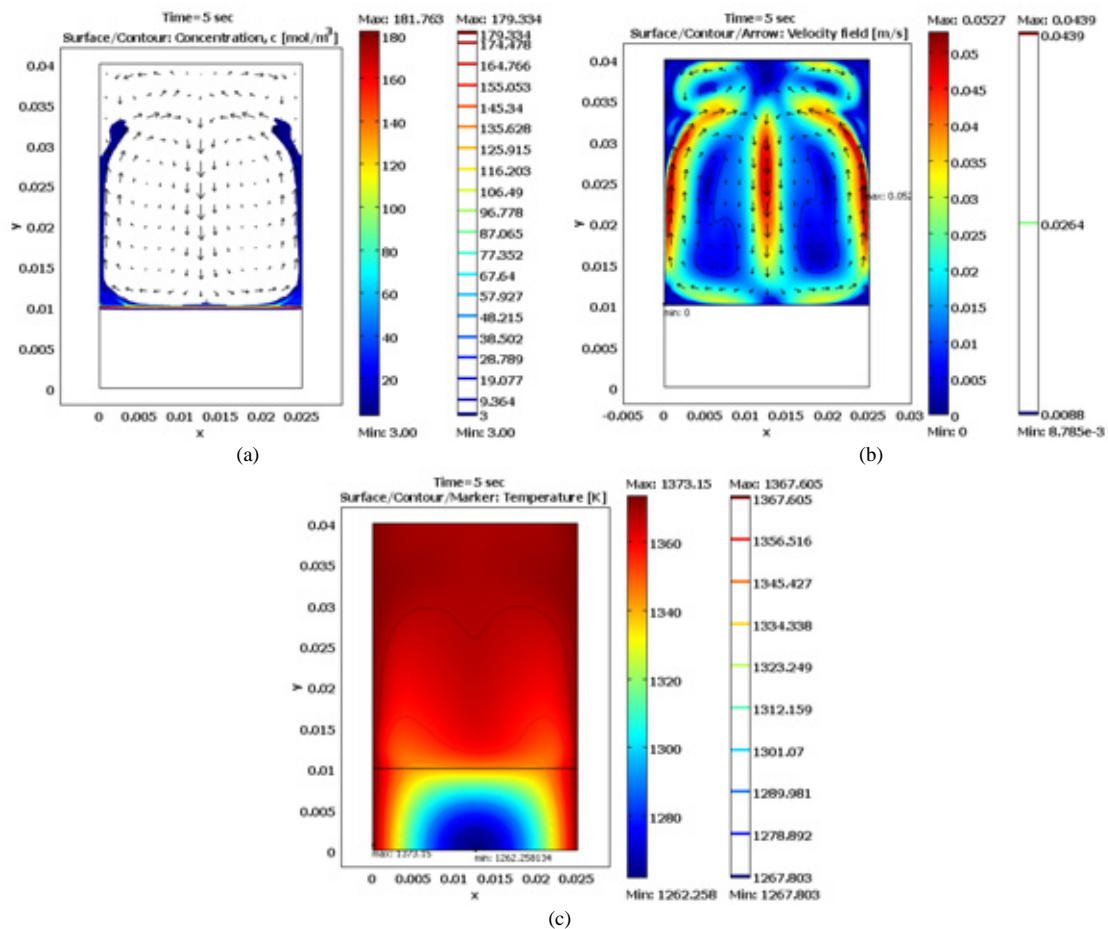
(a)

(b)

(c)

Figure 3. Results obtained after 5 seconds

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