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MODELLING OF THE INTERFACE EVOLUTION DURING SI LAYER GROWTH ON A PARTIALLY MASKED SUBSTRATE

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Abstract: High-quality thin Si layers obtained from the solution by epitaxial lateral overgrowth (ELO) can play a crucial role in photovoltaic applications. The laterally overgrown parts of the layer are characterized by a lower dislocation density than that of the substrate. The height and width of the layer depend on several factors, such as the technological conditions of liquid phase expitaxy (LPE), growth temperature, cooling rate and the geometry of the system (mask filling factor). Therefore, it is crucial to find the optimal set of technological parameters in order to obtain very thin structures with a maximum width (high aspect ratio).

This paper presents a computational study of Si epilayer growth on a line-pattern masked silicon substrate from Si-Sn rich solution. To solve this problem, a mixed Eulerian-Lagrangian approach was applied. The concentration profile was calculated by solving the two-dimensional diffusion equation with appropriate boundary conditions. The growth velocity was determined on the basis of gradients of concentration in the border of the interface. Si interface evolution from the opened window was demonstrated.

Keywords: epitaxial lateral overgrowth, liquid-phase epitaxial growth, computer simulations

1. Introduction

Epitaxial lateral overgrowth (ELO) may be a promising technique in photovoltaic applications due to the possibility of producing high-quality Si epitaxial layers on silicon substrates of poor quality. ELO is a technique of crystal growth on a substrate partially covered by a 100nm-thick dielectric mask. By means of a standard photolithography process, opened Si windows are created. It is here that the layer growth begins. After that, it proceeds in the lateral and normal directions, with different growth rates, which depend on the technological conditions of the experimental process. Given ample time, a new epitaxial layer is able to fully cover the masked substrate. The purpose of using a dielectric mask deposited on the growth substrate is to prevent the propagation of dislocations from the substrate. This is the major advantage of ELO, as it reduces the defect density in the new layer [1–3]. To produce epitaxially overgrown layers, it is recommended to use the liquid phase epitaxy (LPE) method, which offers high crystal quality and requires only simple and inexpensive apparatus.

This paper presents a two-dimensional computational study of the epilayer interface evolution in epitaxial lateral overgrowth by LPE. In order to calculate the motion of the interface, the solute concentration in the Si-Sn solution was determined after each time step. The new position of the interface was obtained by calculating the growth rate along the direction normal to the interface. The growth rate was computed from concentration gradients near the growth surface. To solve the moving interface problem, a mixed Eulerian-Lagrangian approach was used. According to this approach, the solid-liquid front was explicitly tracked, while the diffusive transport was solved on a fixed Cartesian grid. This method was presented in detail in [4]. The simulations were carried out in order to obtain the growth rates and the aspect ratio of the epilayer for the given conditions. The concept of the ghost-cell method was used to improve the solute concentration profile near the border of the grown layer.

2. Computational model

A two-dimensional computational domain for ELO growth is shown in Figure 1. It can be seen that the domain consists of two grids: a uniform Cartesian grid, segmented into $N_x \times N\_y$ equal blocks, which stores concentration data; and a moving interface grid which is represented by a Lagrangian set of connected points which change their positions in time according to the calculated growth rates along the direction normal to the interface. The information about the location of the moving points, on the one hand, and the concentration field in the vicinity of the interface, on the other, must be passed between these two grids.

The concentration field of the solute in the computational domain was obtained by solving the two-dimensional diffusion equation in time:

$$\frac{\partial C(x,y,t)}{\partial t} = D\cdot\left(\frac{\partial^2 C(x,y,t)}{\partial x^2}+\frac{\partial^2 C(x,y,t)}{\partial y^2}\right) \tag{1}$$

where $C(x,y,t)$ is the mass fraction of the solute, and D is the diffusion coefficient of the solute taken as $D = 3.0\cdot 10^{-5}\,\mathrm{cm}^2/\mathrm{s}$ after [5]. The initial concentration C_0 for all elements was set as the equilibrium concentration at the starting temperature T_0 and was taken from the phase diagram of the Si-Sn solution. The phase diagram relation was obtained by fitting a polynomial to the experimental points given in [6]. During the growth process, the temperature T decreased with time according to the formula $T = T_0 - c_r \cdot t$, where c_r is the cooling rate (constant)

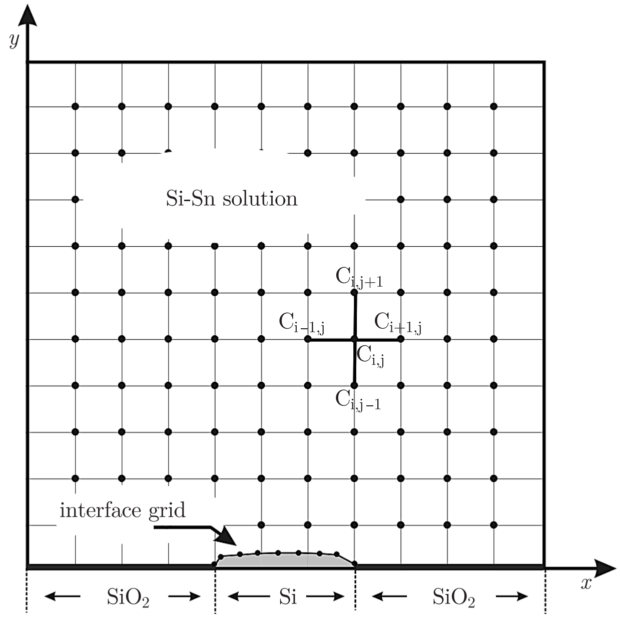

Figure 1. Schematic view of the computational domain used in our simulations. The growth cell consist of 400×400 equal segments of 1μm in size. The opened Si window is 50μm wide. The distance between the two adjacent interface nodes is maintained between 0.6μm and 1.2μm. The thickness of the mask was neglected

and t is the growth time. This signifies that the equilibrium concentration must be calculated at each time step of the simulation. In order to solve Equation (1) to obtain the concentration profiles of Si in the Si-Sn rich solution in time, the central difference method was employed.

The boundary conditions used in the numerical model are as follows. For the two vertical walls ($x=0$; $x=N_x$), the following Neumann boundary condition was used:

$$\left.\frac{\partial C}{\partial x}\right|_{\substack{x=0\\ x=N_x}} = 0 \tag{2}$$

Also, no-flux boundary conditions were used for the calculations in the area between the solution and the oxide mask. This means that neither material deposition on the mask nor solute transfer through the $x=0$ plane take place [1]. The concentration at the upper liquid surface was set as Co. For the grown layer interface, the following equation must be satisfied:

$$D_l \left.\frac{\partial C}{\partial n}\right|_{\text{interf.}} = v_n \left(C_{\text{eq}}^S - C_{\text{eq}}\right) \tag{3}$$

where $C_{\text{eq}}^S = 1$; $C_{\text{eq}}(T)$ is the equilibrium concentration obtained from the phase diagram; and ν_n is the velocity of interface growth. The above condition is known as the Stefan condition. The growth rate ν_n was determined from the gradient of the concentration in the normal direction to the local curvature of the interface on the basis of Equation (3). For this reason, it is crucial to express the concentration field near the layer more accurately, including the real position of the moving grid (Figure 2). In order to improve the concentration field, the sharp-interface method, presented in [7], was used. The main idea behind the method was to apply the ghost concentration to the interface grid points which belong to the solid phase. The ghost concentration was calculated on the basis of equilibrium composition and the known location of the interface.

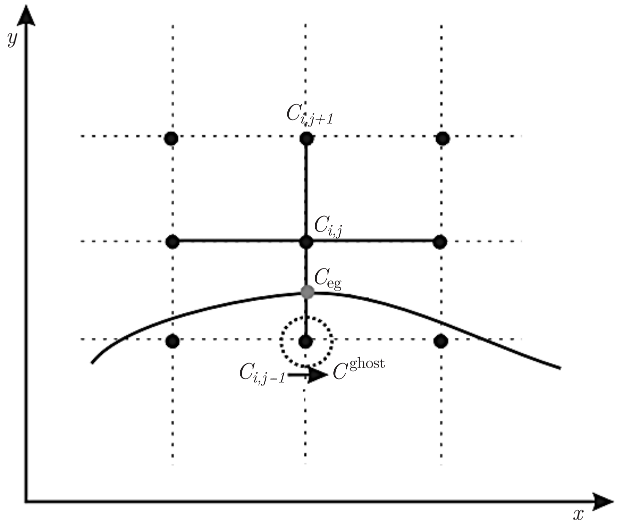

Figure 2. Improvement in the concentration field calculations in the vicinity of the grown layer resulting from the use of the sharp-interface method

After the calculation of the growth rate, each point of the Lagrangian grid is moved to a new location, according to the advection relations:

$$x^{t+1} = x^t + v_x \, dt \tag{4}$$

$$y^{t+1} = y^t + v_y \, dt \tag{5}$$

where v_x and v_y are the x and y components of the growth rate, dt is the time step used in the calculation. As the interface moves, new points must be created to maintain the given distance between two adjacent points of the interface grid.

3. Results and discussion

Computer simulations were carried out for the Si ELO layer grown by LPE on the Si partially-masked substrate. The initial temperature of the system was set at 920°C and 1050°C. The diffusion coefficient was $D = 5.0 \cdot 10^{-5}\,\mathrm{cm}^2/\mathrm{s}$. The calculations were performed for the first few minutes of the real time growth using two different cooling rates (cr), *i.e.* 0.5°C/min and 1.0°C/min.

Figures 3–5 present the results of calculations of the Si concentration field in the Si-Sn solution at the early stage of the growth process. Figure 3 shows the concentration surface after 60s of the simulation with $T_0 = 1050°\mathrm{C}$ and $\mathrm{cr} = 0.5°\mathrm{C/min}$.

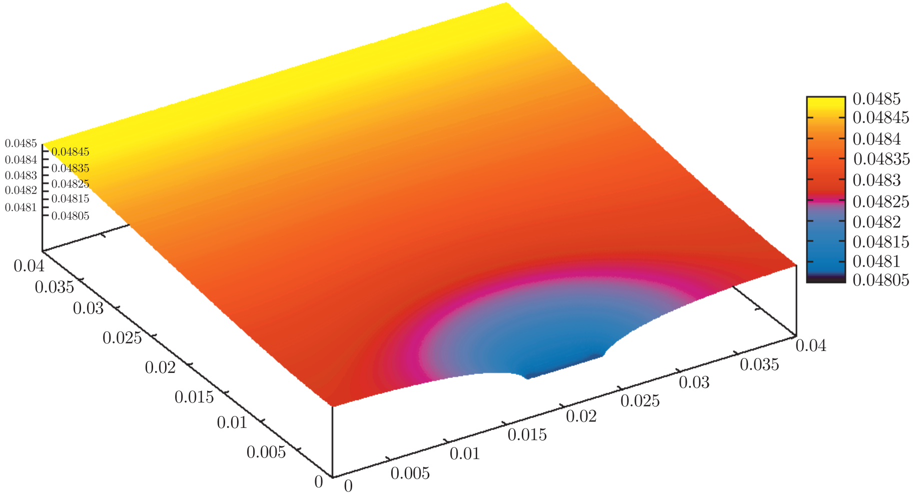

Figure 3. Concentration profile surface of Si in the Si-Sn solution during the growth process

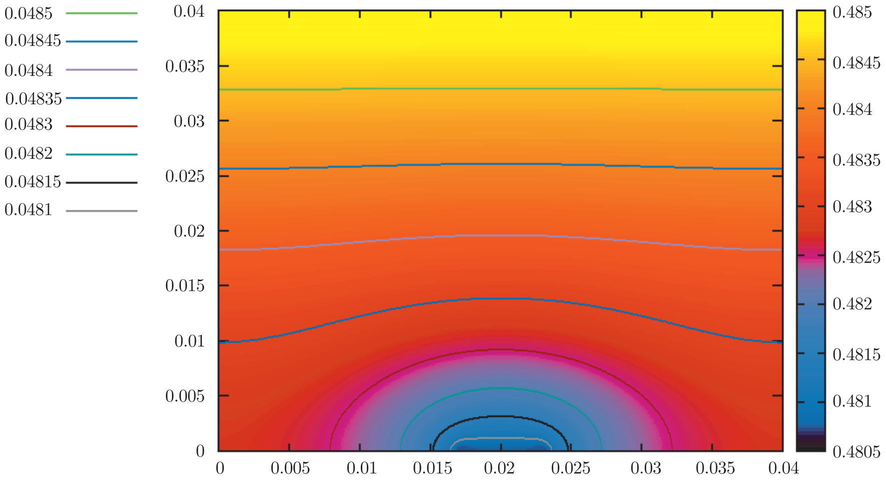

Figure 4. Concentration after 60s of growth. Iso-concentration lines show the direction of the flux of Si in the solution

The temperature of the system decreases with a constant cooling rate. This leads to the growth of the ELO layer and, in consequence, to a decrease in the concentration of solute species in the area of the open window (see Figure 3). The difference between the concentration of Si near and far from the interface drives the flux of the species. It can be seen from the concentration contour map, presented in Figure 4, that the direction of the Si flux is towards the opened Si window. The flux of solute is perpendicular to the iso-concentration lines. It should be pointed out that due to the no-flux boundary condition at the mask, Si species move away from the mask area towards the region of the grown layer. This leads to a higher concentration gradient at the edges of the layer. This is evidenced in Figure 5 by a larger density of contour lines.

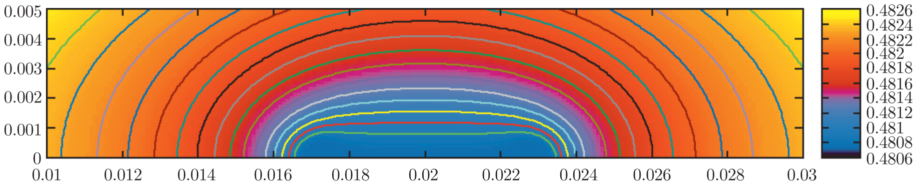

Figure 5. Concentration contour plot in the vicinity of the grown layer after 2 minutes of growth. A larger concentration gradient at the edges of the layer can be observed

As it was mentioned before, the growth rate of the interface was determined on the basis of the concentration gradient from Equation (3). This means that a higher concentration gradient at the edge of the layer leads to faster growth in this region. Also, this can be the main reason for the difference in the value of the growth rate in the lateral and normal directions.

Figure 6 shows the cross-section of the Si ELO layer calculated for 4.5 min of growth, with the initial temperature $T_0 = 920°C$ and a cooling rate of 0.5°C/min. The separation between the lines is 30 s.

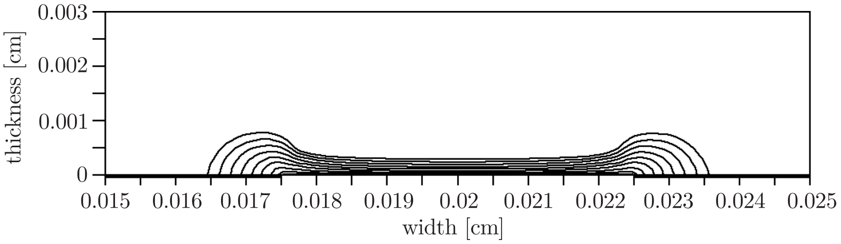

Figure 6. Shape of the ELO layer interface at the first stage of growth. The separation between the lines corresponds to a time interval of 30 s. The initial $T = 920°C$ and cr = 0.5°C/min

It can be seen from Figure 6 that the growth in the lateral direction is significantly larger than in the vertical direction, as evidenced by the distance between any two adjacent lines. After almost 5 min of real-time growth, the thickness of the layer in the flat face is *ca.* 4 μm, whereas the width exceeds 10 μm. This leads to an aspect ratio of almost 2.5 in the early stage of growth. Figures 7–8 show the evolution of the interface of the Si ELO growth for an initial temperature $T_0 = 1050°C$ and for cr = 0.5°C/min and cr = 1.0°C/min, respectively.

Figure 9 illustrates the difference between the growth with an improved concentration profile near the interface and growth without any improvements. The differences in growth became visible after several minutes of growth. Therefore, using a more accurate method for calculating the concentration in the vicinity of the growth interface leads to a more precise calculation of the ELO layer geometry.

4. Conclusions

Two-dimensional computer simulation of the ELO layer growth by LPE was carried out on the basis of a purely diffusional model with moving appropriate

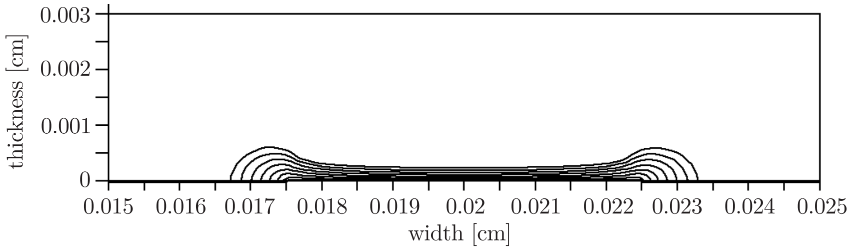

Figure 7. Evolution of the shape of the ELO layer interface. The separation between the lines corresponds to a time interval of 20s. The initial $T = 1050°\mathrm{C}$, $\mathrm{cr} = 0.5°\mathrm{C/min}$, and the total growth time was 160s.

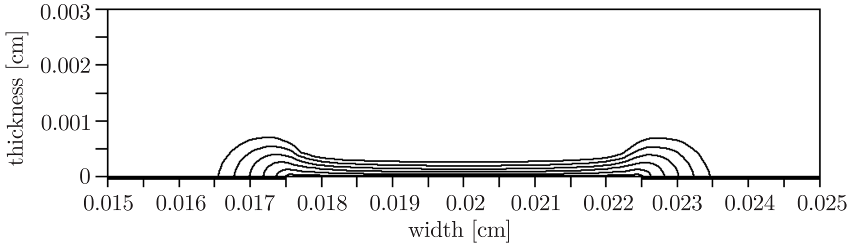

Figure 8. Evolution of the shape of the ELO layer interface. The separation between the lines corresponds to a time interval of 20s. The initial $T = 1050°\mathrm{C}$, $\mathrm{cr} = 1.0°\mathrm{C/min}$, and the total growth time was 2min

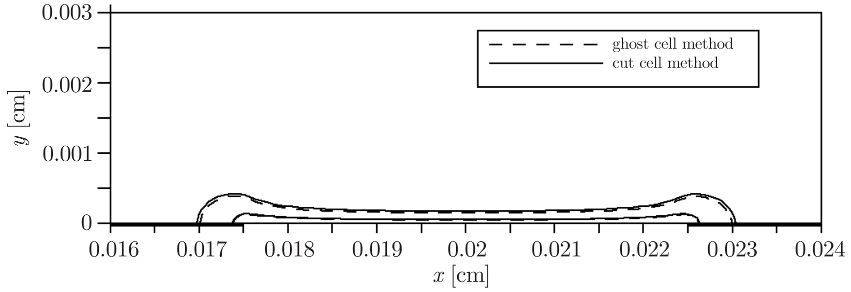

Figure 9. Difference between the epilayer growth, as obtained with the ghost-cell calculation method and the simple cut-cell method, respectively. The lines correspond to a time of 1min and 2min

boundary conditions. The calculation of interface growth rate was performed on the basis of the concentration gradient in the normal direction in the vicinity of the surface. The interface evolution during the growth was investigated and the results of calculations for the early stages of the growth process were shown. It should be pointed out that the ELO layer was growing faster in the lateral direction than in the vertical direction due to the geometry of the growth substrate (mask and Si window). Different growth rates were observed in both directions over a short period of growth time. In order to obtain the results for a longer growth time, it might be necessary to take into account the Gibbs-Thomson effect, because of the curved shape of the interface.

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