

MODELLING OF THIN Si LAYERS GROWTH ON PARTIALLY MASKED Si SUBSTRATE

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Abstract: This paper presents a numerical simulation of epitaxial lateral overgrowth of silicon layers from the liquid phase of an Sn solvent. A two-dimensional diffusion equation has been solved and the concentration profiles of Si in a Si-Sn rich solution during the growth have been constructed. The epilayer thickness and width have been obtained from the concentration near the interface.

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

1. Introduction

The Epitaxial Lateral Overgrowth (ELO) technique is used to grow high quality epitaxial layers on partially masked substrates. In this method epitaxial growth begins in windows that are opened in a dielectric mask deposited on a substrate. Then, the growth proceeds in the lateral direction over the mask. The main idea of this technique is to stop propagation of dislocations from the substrate by the dielectric mask and reduce the defect density in the grown layer [1] which is of crucial importance for many electronic devices, especially for photovoltaic applications.

To obtain epitaxially overgrown layers a Liquid Phase Epitaxy (LPE) may be used which offers high crystal quality due to the use of low-cost and simple apparatus. For this reason many research works focus on producing thin films by LPE. Moreover, some computational studies have been conducted in order to better understand the fundamentals of growth, kinetics, morphology of LPE [2, 3] and mechanisms of ELO by this method [4–6].

In this work we present numerical calculations of ELO of Si on a line-pattern masked Si substrate from a Si-Sn solution using the LPE technique basing on the results obtained in our experimental work on liquid phase epitaxy in an Ar ambient

and using the approach proposed by Kimura *et al.* [2] and Yan [5]. A special computer program for growth simulations from the melt has been developed.

2. Experimental

Epitaxial Lateral Overgrowth by Liquid Phase Epitaxy experiments which allowed simulation parameters to be determined were carried out in a standard horizontal slider boat system. We used (111) oriented Si substrates with line-seed patterns oriented along the $\langle 011 \rangle$ direction as growth substrates and (100) Si as source wafers. As a solvent, pure (5N) tin was used. The initial temperature was equal to 920°C for 1 h. The cooling rate was equal to $1^\circ\text{C}/\text{min}$. More details of the experimental method as well as the results in Ar ambient can be found in [7, 8].

3. Numerical simulations

A two-dimensional region of a size equal to 0.1mm in both directions has been chosen as a simulation domain. Due to the solution's symmetry, only the part schematically shown in Figure 1 has been taken into consideration.

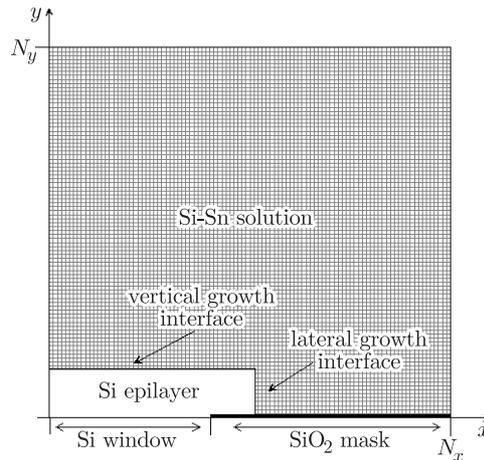


Figure 1. The growth cell part used in numerical calculations. The Si window and SiO_2 mask are $50\ \mu\text{m}$ and $100\ \mu\text{m}$ wide, respectively

A uniform mesh has been constructed. At the beginning, initial concentration C for all elements has been set as equilibrium concentration at the starting temperature T_0 based on phase diagram of the Si-Sn solution:

$$C(x, y, t = 0) = C_0. \quad (1)$$

In the numerical simulation the temperature T of the system decreases with time to supersaturate the solution:

$$T = T_0 - c_r \cdot t, \quad (2)$$

where c_r – the cooling rate (const.), and t – the growth time.

After each time increment τ the concentration profile was calculated.

During the simulation process the 2D diffusion equation has been solved numerically. The fluid flow contribution to mass transport in the liquid is neglected.

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right), \quad (3)$$

where D denotes the solute diffusion coefficient in an Sn solution.

Replacing the left and right sides of Equation (3) with first order forward difference and central difference formulas respectively, we obtain a finite difference equation scheme for Equation (3):

$$\frac{C_{i,j}^{n+1} - C_{i,j}^n}{\Delta t} = D \left[\frac{C_{i-1,j}^n - 2C_{i,j}^n + C_{i+1,j}^n}{\Delta x^2} + \frac{C_{i,j-1}^n - 2C_{i,j}^n + C_{i,j+1}^n}{\Delta y^2} \right], \quad (4)$$

which for $\Delta x = \Delta y = d$, $\Delta t = \tau$ and simple rearrangements in Equation (4) can be written as:

$$C_{i,j}^{n+1} = C_{i,j}^n + \frac{D \tau}{d^2} (C_{i-1,j}^n + C_{i+1,j}^n + C_{i,j-1}^n + C_{i,j+1}^n - 4C_{i,j}^n), \quad (5)$$

where i, j denotes the segment number in the X and Y direction, and n is the time step of the simulation.

Equation (5) has been used in computing concentration in the i, j -th segment of the mesh each time after increment τ . A serious limitation of the explicit approach used for computations are the stability constraints of choosing d and τ . In our case the restriction is as follows:

$$\frac{D \tau}{d^2} < \frac{1}{4}. \quad (6)$$

For a diffusion coefficient D equal to $3.0 \cdot 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ (from [2]) Equation (6) leads to very small τ which results in long computer calculations. For that reason it is very important to choose optimal values of d and τ [9] The mesh configuration has been set in our computer program, τ is calculated automatically from Equation (7):

$$\tau = 0.49 \cdot \frac{d^2}{2D}. \quad (7)$$

The boundary conditions used in the numerical model are as follows:

For the two vertical symmetry planes ($x = 0$; $x = N_x$) and for upper liquid surface ($y = N_y$) we have used the Neumann boundary conditions:

$$\left. \frac{\partial C}{\partial x} \right|_{x=0} = 0, \quad \left. \frac{\partial C}{\partial y} \right|_{y=N_y} = 0. \quad (8)$$

No flux boundary conditions have been used for calculations in the area between the solution and oxide mask, either. It means that there is neither material deposition on the mask nor a solute transfer through the $x = 0$ plane [4].

For lateral interface we have assumed the simple boundary condition shown below:

$$D \frac{dC}{dx} = C_{\text{eq}}, \quad (9)$$

where C_{eq} can be obtained from the phase diagram of Si in the Si-Sn solution. As for the vertically growing surface, the following equation has been used:

$$D \frac{dC}{dx} = q_v (C - C_{\text{eq}}). \quad (10)$$

Surface reaction constant q_v , for a vertical surface has been determined in this study by using experimental data. The above condition means that the diffusive flux

of Si species to the surface equals the rate of destruction due to the chemical reaction on that surface. The growth rate in our model has been determined from the solute gradient near the appropriate surface [2]:

$$G(t) = \frac{\rho D}{\rho_c} \frac{1}{1-C} \frac{\partial C}{\partial y}, \quad (11)$$

where ρ and ρ_c denote the solution and crystal density, respectively.

4. Results and discussion

We have simulated the concentration profiles and lateral growth of Si with different growth times and cooling rates using our computer program. Diffusion coefficient $D = 3.0 \cdot 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ has been chosen for our simulations from [3]. The solution density in liquid has been taken as $6.29 \text{ g} \cdot \text{cm}^{-3}$ [10]. The initial temperature of the system in numerical experiments has been the same as in the experimental results. The surface reaction rate for vertical interface has been chosen as $q_v = 1.0 \cdot 10^{-4} \text{ cm/s}$. This value corresponds to the Si ELO layer growth rate prediction from the results of our experimental work.

Figure 2 presents the concentration profile of Si in the Si-Sn solution in the case under consideration. The cooling rate has been set as 1.0°C/min . As can be seen from Figure 2, the solute flows into the opened window in the growth substrate. Moreover, it can be seen from the contour profile shown in Figure 3 that the solute concentration gradient near the laterally growing surface is slightly larger than the gradient near the vertical surface. It means that the growth rates for both interfaces are different.

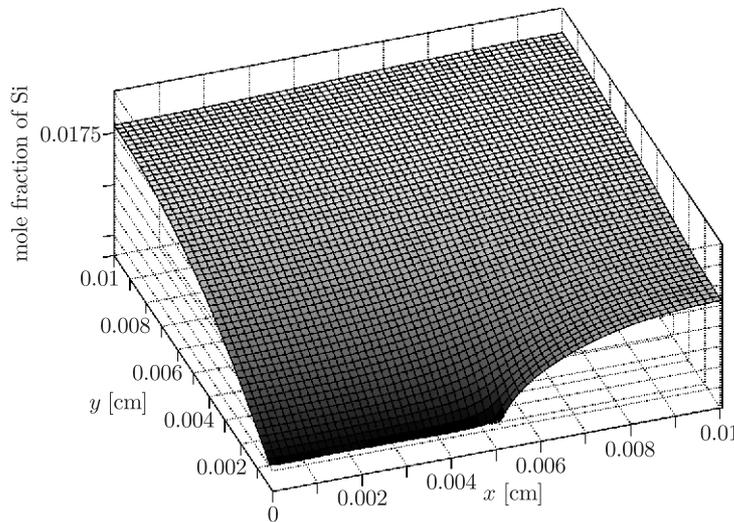


Figure 2. Concentration profile surface of Si in Si-Sn rich solution during simulation

Figure 4 presents the growth rates as a function of time obtained as a result of computer simulations. As can be seen, the growth rate increases at the beginning of the process, and after a few minutes remains approx. constant. On the basis of this fact, the size of the new grown layer can be determined.

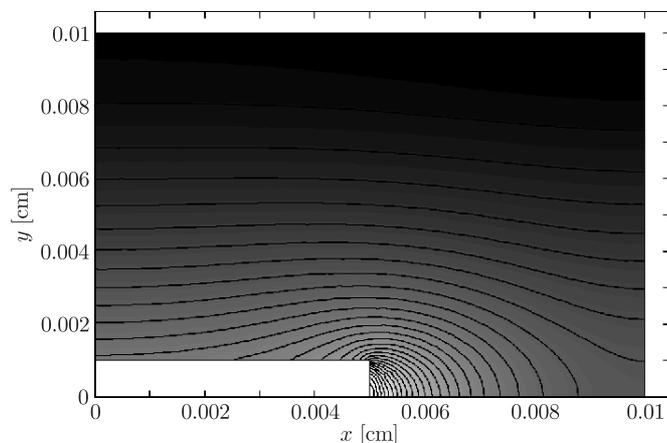


Figure 3. Concentration field contour plot after few minutes of simulation

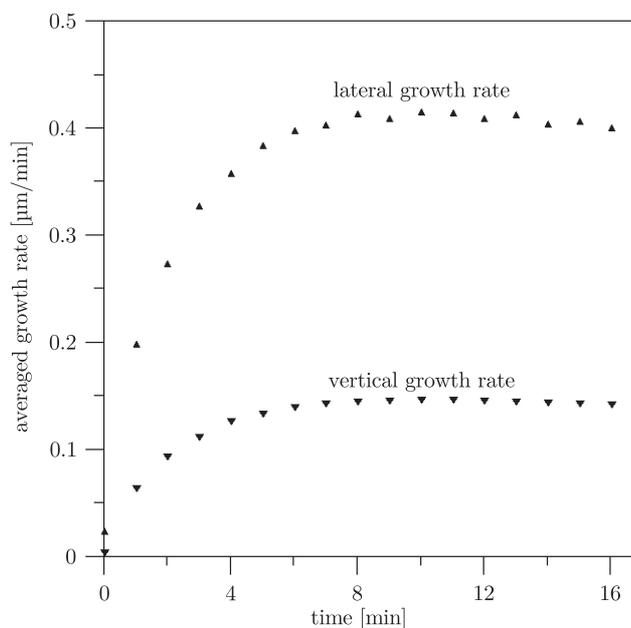


Figure 4. Epitaxial layer simulated considering estimated reaction constants for vertical and lateral surface

5. Conclusions

Computer simulations based on a diffusion-reaction model with parameters obtained on the basis of the LPE experimental work results have been carried out. Our approach could be a good solution to reduce the number of necessary experiments, and can optimize some parameters for carrying them out. However, more parameters, such as mask orientation or pattern substrate orientation as well as the interface movement during the growth, should be considered in numerical calculations in order to obtain a more precise and accurate model. As there are more results of the experimental work carried out by our group, we plan to take them all into consideration in the future.

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