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Computer Modeling in Cost-Efficient Solar Cell Production Technology

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1. Introduction

The progress of the Liberal Capitalism in the last years led to faster use of the World energy resources [24, 21]. Because of the fast energy consumption the conception of sustainable development has been formulated [20]. One of the suggested directions of the development is the idea of green economy [9], low carbon growth [4, 25, 28]. Because of using a great amount of energy the research on the optimization of this consumption have been started [3]. Considering Sun as one of the biggest energy source and convert this energy into biomass the main renewable energy resource can be obtained. On the other hand, production biofuel from biomass leads to increase a food price [23]. More suitable for environment is biomethanization process in specially developed reactors [14] or converting biogas from municipal waste landfills [26]. Another solution is thermal utilization of other wastes[22]. One of the biggest possibilities of production energy from renewable sources is photovoltaics. More than 80% of the current solar cells production requires cutting of large silicon crystal. During this process about 50% of the material is lost. Due to this fact, sawing costs comprise 29% of the total wafer production cost, and thus contribute considerably to the total module cost [13]. The technology which could avoid the sawing step of the cell production, can be a method for future developing cost-efficient solar cells. One of the promising technique in this application is Epitaxial Lateral Overgrowth (ELO) technology with Liquid Phase Epitaxy (LPE) equilibrium method [2, 1, 5]. Using thelow-cost and simple apparatus allows to

produce high quality Si epitaxial thin films on silicon substrates with poor quality.

ELO is the crystal growth technology in which layer starts to crystallize inside the narrow Si windows opened in dielectric mask with using standard photolithography process. Then it proceeds in lateral and normal direction with different growth rates. The major point of ELO is to reduce defect density in the grown layer. More detailed description of the ELO technology as well as LPE method can be found in papers [32, 31, 18, 11].

With the rapid progress in computer technology, simulations and modeling become the new scientific practice which can be compared to the traditional experimental research. Increasing number of simulation works can be observed also in the area of epitaxial growth methods. However, there arestill not many papers concerningthin Si films growth modeling. Existing models are based on the assumption that growth is diffusion and kinetic limited. Kinetic coefficient is determined in experimental work and added into the model [29, 15, 16].

The computational model presented in this work is based on the assumption that growth is diffusion–controlled and mass transfer is the main process to reach thermodynamic equilibrium between the solid and liquid phase on the interface. For this reason, the concentration gradients in the vicinity of the grown interface determine the growth rate and in consequence shape of the surface. Modeling this problem, generally known as Stefan's problem, requires the simultaneous solution of the mass transport to the substrate and the interface displacement. It should be emphasized that geometry of the calculation domain changes during the process. In order to solve this complex problem the special computer software was implemented in Matlab code.

2. Numerical simulation model

The main idea of the simulation model developed for the epitaxial growth of Si layer on silicon substrate is to calculate growth rate of the interface on the basis of concentration gradients in the vicinity of the moving surface. Two-dimensional computational domain consists of two main parts. Firstone keeps information about Si concentration in the solution. This is liquid phase of the system. Second part is moving interface

grid which represents interface of the layer. Interface nodes changetheir position in time according to the calculated growth rates in the normal direction to the interface. Information about the position of moving grid on the one hand, and concentration field in the vicinity of the interface on the other hand is passed between these two grids. The concept of the model is as follows.

During the growth process, the temperature T decreases with time according to the formula $T = T_0 - c_r \cdot t$ where $c_r$is the constant cooling rate and t is the growth time. The initial concentration C_0 for the liquid solution, set as equilibrium concentration at the starting temperature T_0, is obtained from the phase diagram relation of Si in binary solution [19, 10].

As the temperature of the system decreases, new concentration profile is set according to the formula (1).

$$\frac{\partial C(\xi,t)}{\partial t} = D_{Si}\nabla^2 C(\xi,t), \tag{1}$$

where $C(\xi, t)$ is the mass fraction of the solute and D is the diffusion coefficient of solute, which can be taken from [12]. Boundary conditions of the model for vertical walls of the system and the oxide mask have been chosen asno flux Neumann boundary condition (2):

$$\left.\frac{\partial C}{\partial n}\right| = 0. \tag{2}$$

For the interface following equation has to be fulfilled:

$$D_{Si}\left.\frac{\partial C}{\partial n}\right|_L = v_n \cdot (C^s_{eq} - C_{eq}), \tag{3}$$

where C^S_{eq} and $C_{eq}(T)$ are the equilibrium concentrations of components at the interface on the sides of solid and liquid phases. Growth rate $v_n$is determined from the gradient of concentration in normal direction to the local curvature of the interface. On the basis of the calculated growth rate shift of the interface in each time step is determined.

More detailed description of the model can be found in our previous calculation papers [8, 7].

3. Finite Element Solution Method

The finite element method is used to solve the moving boundary problem defined above. The modeled Si growth process involves mass transport in the liquid and equilibrium at the moving interface. These types of problems can be generally solved with the use of Front Tracking Methods [30, 17, 27]. Most of them use uniform mesh to calculate concentration profiles. In our case a non-uniform adaptive mesh is used to obtain efficient meshing in high gradient regions. It leads to very precise concentration profiles in the area of grown interface especially on the edges of the layer. Fig. 1 presents example of using adaptive meshing for the domain with three opened Si windows. Higher solution grid can be seen in the area of moving interface. This conception minimize the number of computation nodes with maintaining high accuracy of the solution.

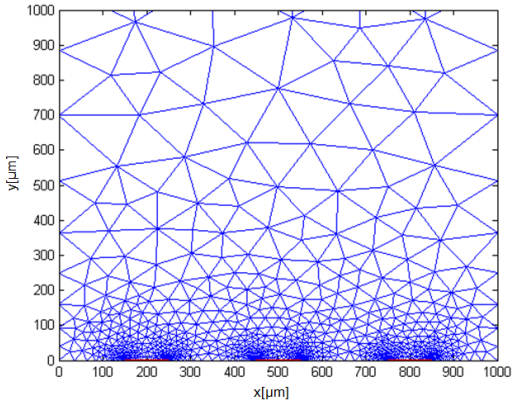

Fig. 1. Grid structure of the calculation domain
Rys. 1. Struktura siatki w domenie obliczeniowej

The computational procedure consists of the following main steps:

1. Set initial computational geometry,
2. Set initial concentration profile for T_0,
3. Generate triangle mesh for the given geometry,
4. Decrease temperature T and calculate equilibrium concentration C_{eq},
5. Calculate gradients of concentration and growth rate,
6. Calculate growth thickness and determine interface shape,
7. Calculate new geometry and return to step 3.

4. Results and discussion

In our previous modeling work [6] evolution of the interface during thin film layer growth for one window domain was presented. This paper is focused on the distance dependence between two adjacent windows during epitaxial growth. Similar to the previous studies, computations were performed using diffusion coefficient of Si in tin equals $D = 5.0 \cdot 10^{-5}$ cm^2/s [12]. Size of the domain was 1000 μm x 2000 μm. The growth process was started from the temperature of 920ºC and proceeded with constant cooling rate equals 0.5ºC/min.

Figs. 2 and 3 show concentration surfaces of Si in Si-Sn binary solution of the whole domain. Because of the crystallization process, depletion of the Si atoms near the growth substrate can be observed. The difference in concentration of Si near the interface and in faraway from it force flux of the Si atoms to the interface.

Comparing profiles presented in Figs. 4and 5with the profilesobtained for one window [7], similarity in the area of growth substrate can be observed. Stream of solute is perpendicular to the isoconcentration lines. Due to no flux boundary condition for the mask region all Si species move from the mask area towards the region of the grown layer. It leads to higher gradient concentration in the region of layer's edges and in consequence to higher growth rate in that region.

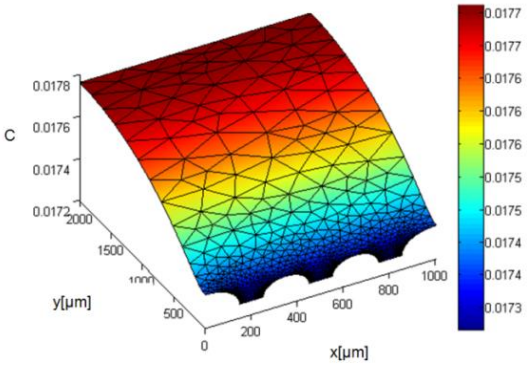

Fig. 2. Concentration plot of Si in the solution for growth substrate consisted of three opened Si windows

Rys. 2. Powierzchnia koncentracji Si a roztworze w przypadku podłoża wzrostowego zawierającego trzy okna krzemowe

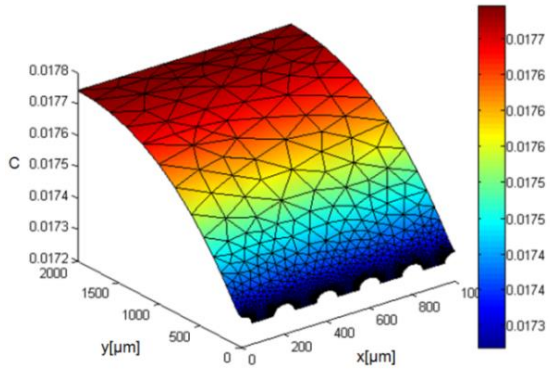

Fig. 3. Concentration plot of Si in the solution for growth substrate consisted of five opened Si windows
Rys. 3. Powierzchnia koncentracji Si a roztworze w przypadku podłoża wzrostowego zawierającego pięć okien krzemowych

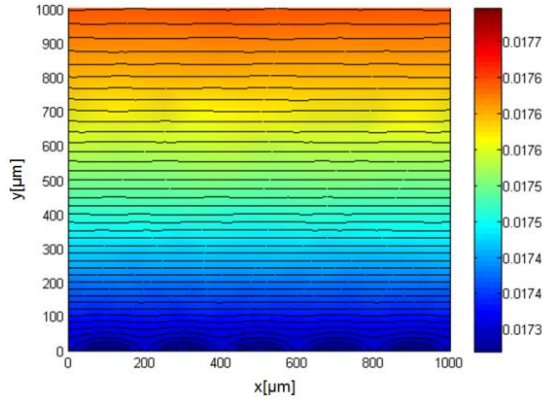

Fig. 4a. Concentration contour plot of Si in the solution for the geometry of several Si widows obtained for computational domain
Rys. 4a. Wykres konturowy Si w roztworze dla geometrii zawierającej kilka okien uzyskany dladomeny obliczeniowej

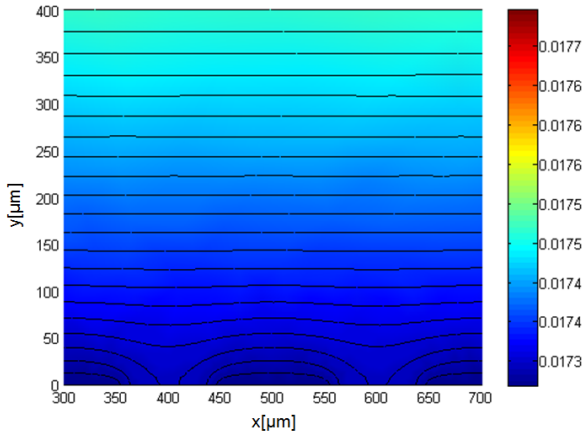

Fig. 4b. Concentration contour plot of Si in the solution for the geometry of several Si widows obtained for area of 400 x 400 µm of the same domain
Rys. 4b. Wykres konturowy Si w roztworze dla geometrii zawierającej kilka okien Si w obszarze 400 x 400 µm

The simulation results of the lateral growth rate in function of time for three different substrate geometry have been shown in Fig. 5. Similar to our previous results for one window geometry [6] the growth rate is rising for the first minutes of growth and then becomes constant due to size of the domain. Fig. 5 shows also dependence of lateral growth rate on the geometry of the substrate. The highest growth rate is for the geometry in which most of the substrate is covered by dielectric mask. It means that if the distance between two adjacent windows is bigger the more species flow from the mask region to the interface of the layer. It leads to the higher concentration gradient and in consequence to higher growth rate. It is also visible in Fig. 6 in which ratio of lateral to vertical growth rate (Aspect ratio – *Ar*) for different substrate geometry was shown.

As it can be seen in Fig. 5 aspect ratio decreases with decreasing the amount of the substrate surface covered by dielectric mask. It means that aspect ratio decreases with the decreasing distance between adjacent window. It is significant observation for the stage of creation growth substrate in photolithography process.

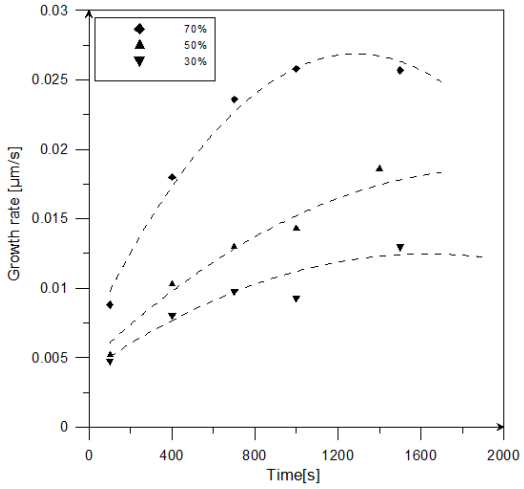

Fig. 5. Growth rate dependence on time for three substrate geometries with different mask-to-window ratio
Rys. 5. Wykres zależności szybkości wzrostu od czasu dla trzech geometrii podłoży o różnym współczynniku wypełnienia podłoża

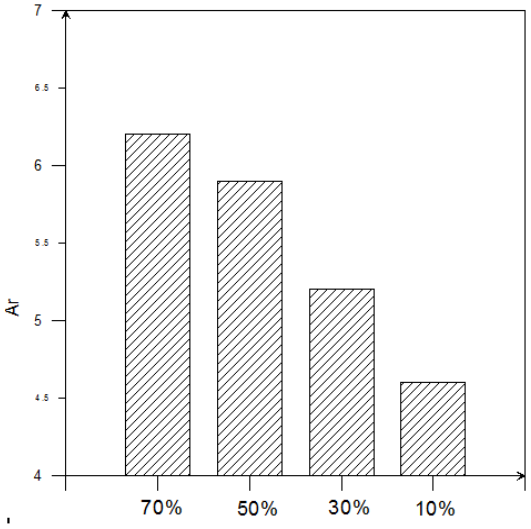

Fig. 6. Aspect ratio dependence on the mask-to-window ratio of the growth substrate
Rys. 6. Wykres zależności parametruaspect ratio od współczynnika wypełnienia podłoża

5. Conclusions

Computer simulation of the epitaxial layer growth from the liquid phase was used to analyze thin film growth on masked substrate. Concentration profiles for different substrate geometry was calculated as a consequence of species transport due to crystallization on the surface. Growth rates on the basis of concentration gradients in the vicinity of the interface for different substrate geometry were shown. Obtained results show the correlation of the lateral growth rate with substrate area covered by mask and in consequence with distance between adjacent windows. Increasing this distance leads to increase Si flow from the area of oxide mask to the grown layer.In consequence it leads to higher concentration gradient and faster growth in this region. It is very significant in the process of preparing growth substrate for epitaxial growth for photovoltaic applications.

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Komputerowe modelowanie w technologii produkcji ekonomicznych ogniw słonecznych

Streszczenie

W artykule przedstawione zostały rezultaty symulacji lateralnego wzrostu epitaksjalnego (ELO – Epitaxial Lateral Overgrowth) przeprowadzonych dla krzemowych podłoży wzrostowych o różnych współczynnikach wypełnienia maski (mask-to-window ratio): 70%, 50%, 30% oraz 10%. Zastosowano przy tym następujące parametry: wymiary domeny: 1000 μm × 2000 μm, szybkość chłodzenia: 0,5ºC/min, temperatura początkowa: 920ºC.

Przedstawiono przykładową domenę obliczeniową oraz wygenerowaną siatkę numeryczną. W celu zwiększenia precyzji obliczeń w obszarach dużych gradientów koncentracji zastosowano zagęszczenie siatki. Dla wybranych geometrii domen przedstawiono profile koncentracji.

Zbadano wpływ geometrii obszaru na kształt pola koncentracji, określającego strumienie masy. Zwiększenie powierzchni krystalizacji składnika spowodowało ukształtowanie się linii stałej koncentracji w objętości roztworu,

charakterystyczne dla standardowej metody LPE. Kierunek przepływu Si w objętości jest prostopadły do powierzchni podłoża na całej jego długości. Natomiast przy powierzchni podłoża, na stosunkowo niewielkiej odległości, tworzy się warstwa roztworu, w której linie stałej koncentracji układają się wokół okien Si. Grubość tej warstwy zależy od stopnia wypełnienia i maleje wraz ze wzrostem liczby okien w obszarze domeny. Sąsiadujące ze sobą okna stanowią dla siebie konkurencję pod względem obszaru krystalizacji: tym większą, im bliżej siebie są umiejscowione. Przyczynia się to bezpośrednio do zmniejszenia szybkości wzrostu w kierunku lateralnym przy niewielkiej zmianie wartości szybkości w kierunku normalnym. Skutkuje to również zmniejszeniem wydłużenia względnego otrzymywanych warstw.

Z analiz numerycznych wynika, że w celu otrzymania warstw lateralnych o maksymalnym wydłużeniu względnym należy uwzględnić szerokość pasm dielektryka znajdującego się między oknami. Odpowiednie dobranie geometrii podłoża pozwala na uzyskanie możliwie maksymalnych szybkości wzrostu w kierunku lateralnym.