COMPUTER IMPLEMENTATION OF MASS TRANSPORT IN MATLAB ENVIRONMENT FOR MODELING EPITAXIAL GROWTH PROCESS WITH MOVING BOUNDARY PROBLEM

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Abstract: Due to the possibility of producing high quality and low cost silicon substrates the Epitaxial Lateral Overgrowth technology may find its application in the photovoltaic industry. However, a lateral growth process depends on many technological parameters such as the temperature of the system, the cooling rate, the solvent or the geometry of the mask. For this reason finding optimized settings for these factors in experimental research is difficult and time consuming. Numerical analysis of the growth process leads to better understanding of the fundamentals of the growth process. For this reason a computational model of epitaxial growth was proposed. This paper focuses on the accuracy of the numerical solution of the mass transport process during epitaxial growth. The method was implemented in the Matlab environment for the moving boundary application. The results of the calculations are presented.

Keywords: moving boundary problem, computational modeling, epitaxial growth

1. Introduction

Epitaxial Lateral Overgrowth (ELO) is the crystal growth technology in which the thin film layer crystallizes on a substrate covered by a dielectric mask with opened windows in it. The major point of ELO is to reduce the defect density in the grown layer. A more detailed description of the ELO technology as well as the LPE method can be found in the papers [1–4].

The numerical model proposed for the solution of the epitaxial lateral overgrowth process from the liquid phase assumes a two dimensional computational domain. The major point in this approach is the geometry of the domain which has to change in time because of the moving interface during the crystallization process. For this reason the domain consists of two grids. One of them is

a triangular mesh which stores information about the concentration field in the domain. The second grid represents the interface of the moving front. Unlike to other simulation works [5–7] the assumption of the proposed model is that the epitaxial growth is only diffusion controlled and the mass transfer is the main process to reach thermodynamic equilibrium between the solid and liquid phase on the interface. The growth rate of the layer interface is obtained from the gradient of concentration of the solute atoms in front of the interface. For this reason the precision of calculation of the gradients is the most important factor of the simulation process. A more detailed description of the proposed model can be found in other papers of the author [8–10].

In this paper the attention was paid to this stage of the process in which the mass transport of the solution is calculated. The solution of the mass transport problem including the moving boundary problem was implemented in the Matlab software. The advantage of the chosen environment is the possibility of using an adaptive grid method which leads to a higher accuracy of the solution in the interface area.

2. Basic conception of approach

The main concept of the developed model is to calculate the silicon mass transport from the Si-Sn liquid into the Si substrate. The simulation has to be done including the moving boundary of the Si layer interface due to the crystallization process which occurs during epitaxial growth.

The overall computational procedure of the developed application consists of the following steps:

1. Set the initial parameters of the simulation and calculation domain.
2. Set the boundary conditions for the interface.
3. Generate a triangular adaptive mesh for a given geometry of the domain.
4. Calculate the mass transfer of Si in the liquid solution on the triangular mesh and the growth rates in the vicinity of the epitaxial interface.
5. Interpolate the Si concentration profile from the PDE triangular mesh to the rectangular Cartesian grid.
6. Modify the position of the interface on the basis of the calculated growth rates.
7. Update the geometry of the domain and return to step 3.

Attention in this paper was paid to the calculations of the concentration profiles on the triangular and rectangular grid. However, the whole process has been briefly described in order to better understand this step of modeling.

2.1. Geometry of the domain and boundary conditions

The polygon object which represents a set of points was used to draw the geometry of the calculation domain with the use of command line functions. Information about the coordinates for each point is stored in the geometry matrix. It consists of two kinds of elements. The first one is fixed and determines the walls and mask regions of the growth substrate. The second element is the moving one

which changes its position in time. These elements represent the moving front of the layer. Due to the interface movement the geometry matrix has to be updated after each time step of the calculation process. An example of the domain with few elements as well as the geometry matrix are shown in Figure 1.

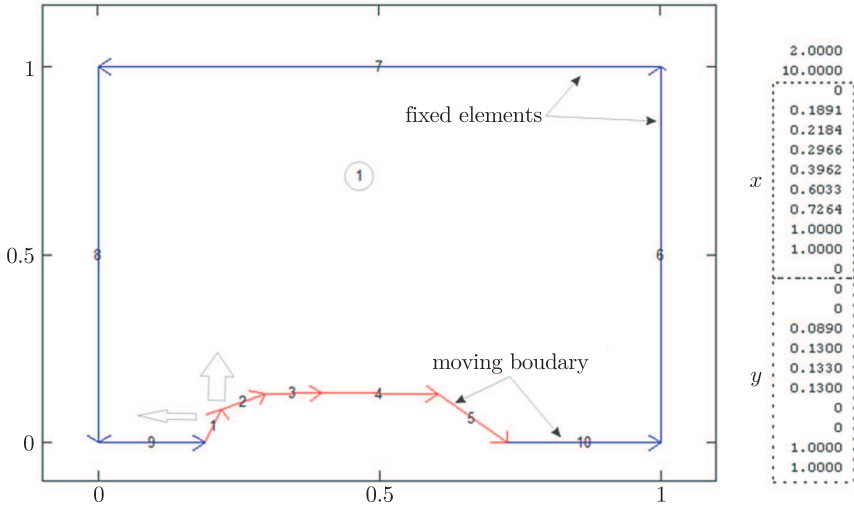

Figure 1. Example of geometry and boundary domain

The Neumann boundary conditions were used for fixed elements. A similar no flux condition was used for elements which represent the dielectric mask. For moving elements, the Dirichlet condition was set in order to control the equilibrium concentration of Si on the interface. The boundary conditions were specified in a matrix which was created for the described geometry matrix.

In the Matlab environment the Dirichlet boundary condition is:

$$hu = r \tag{1}$$

where h in general is a function of x, y, u is the solution and r is the value of the solution on the boundary segments. In the presented approach $h = 1$. The generalized Neumann boundary condition equation is:

$$\vec{n} \cdot (c \cdot \nabla u) + qu = g \tag{2}$$

where $\vec{n}$ is the outward unit normal, g and q are functions defined on the boundary segments and u is the solution. In order to obtain the isolation condition for vertical walls and mask regions coefficients q and g were set equal to zero.

2.2. Mass transfer and interface evolution

On the basis of the given geometry and boundary conditions a triangular mesh was created. Minimal regions were triangulated into subdomains and border segments and boundary segments were broken up into edges. The mesh refinement method was used for higher precision of the calculation in the moving interface area.

The mass transport equation had to be solved to obtain the concentration profile on a given mesh. In the Matlab environment parabolic PDE is given by the following equation:

$$d\frac{\partial u}{\partial t} - \nabla \cdot (c \cdot \nabla u) + au = f \tag{3}$$

For the simulation of epitaxial growth from the liquid phase, the coefficients were set as follows: $d = 1$, $a = 0$, $f = 0$. Parameter c is the diffusion coefficient of the solute in the solution, and u is the concentration of the solute in the solution.

On the basis of the calculated profiles the growth rate in the normal direction to the interface can be determined and therefore the layer interface evolution can be obtained. The process of epitaxial lateral overgrowth modeling requires high precision of concentration profile calculations in the vicinity of the growing interface. It should be emphasized that calculations of the layer interface movement have to be done at the same time as the mass transport calculation. For this reason, it is necessary to use a rectangular grid for keeping the values of concentration profiles after each time step of the simulation process. The results of calculations of the concentration profiles with the use of the interpolation method for triangular and rectangular meshes are shown in the next section.

3. Results and discussion

The main stage of the simulation process was the calculation of the concentration profile with the moving boundary problem included. A computer implementation of the model for the irregular domain had to be verified on the basis of the known analytical solution. Special attention was paid to the size of the triangular and regular mesh. The efficiency of the used method was compared to the results obtained with the use of the standard Euler and Crank-Nicholson scheme.

Figure 1 shows the computational domain which was used to verify the developed modules. A triangular mesh with 10^2 elements was generated. The Dirichlet boundary condition was used on the borders of the domain. An analytical solution for the presented area can be obtained from Equation (4):

$$u = e^{-2\pi^2 Dt} \cos(\pi \cdot x) \sin(\pi \cdot y) \tag{4}$$

where $D = 1$, $\Omega = [-1,1] \times [-1,1]$ and u is the concentration profile.

The concentration profile calculated on the basis of Equation (4) and triangular grid (Figure 2) is presented in Figure 3. As the domain geometry changes in time, the calculated profile was interpolated on a Cartesian rectangular grid. Examples of the results of the interpolation with different sizes of rectangular grids are shown in Figures 4(a) and 4(b).

As can be seen in Figure 4(a) the regular grid size is not sufficient, especially for the borders. For this reason it was necessary to increase the number of nodes in the regular grid. A detailed error analysis with the use of Equations (5)–(7)

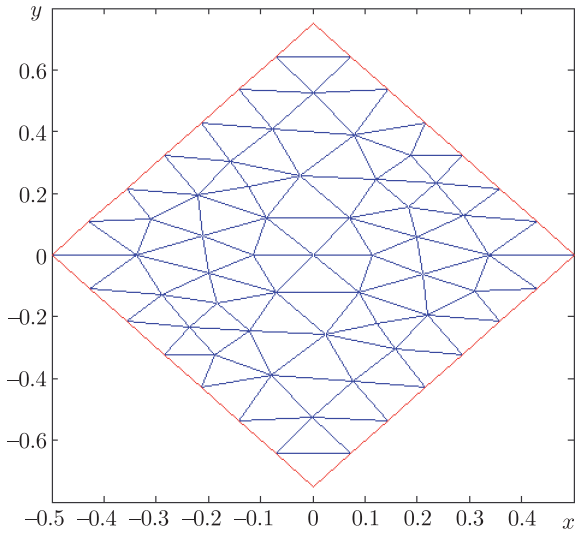

Figure 2. Calculation domain with triangular mesh, number of elements $\sim 10^2$

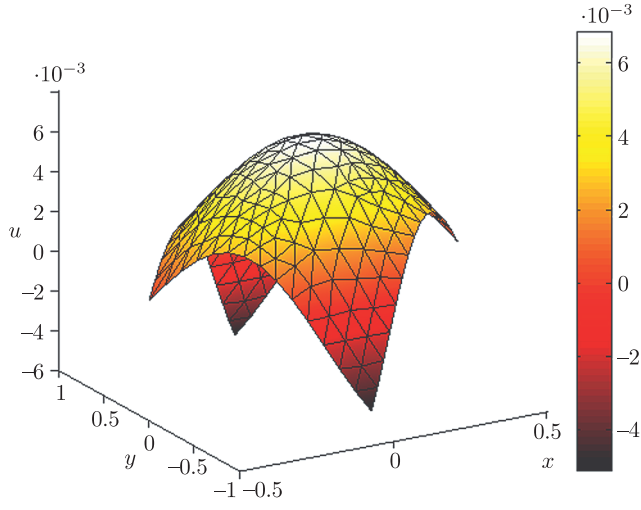

Figure 3. Concentration profile obtained for the domain presented in Figure 1

allows obtaining an optimal size of the triangular grid as well as the Cartesian rectangular grid:

$$L_1 = \frac{1}{m}\sum_{i=1}^{m}|e_i| \tag{5}$$

$$L_2 = \left[\frac{1}{m}\left(\sum_{i=1}^{m}|e_i|^2\right)\right]^{\frac{1}{2}} \tag{6}$$

$$L_{\max} = \max|e| \tag{7}$$

where m determines the amount of data, e_i determines the error of the numerical solution compared to the analytical one for a given (x,y) node.

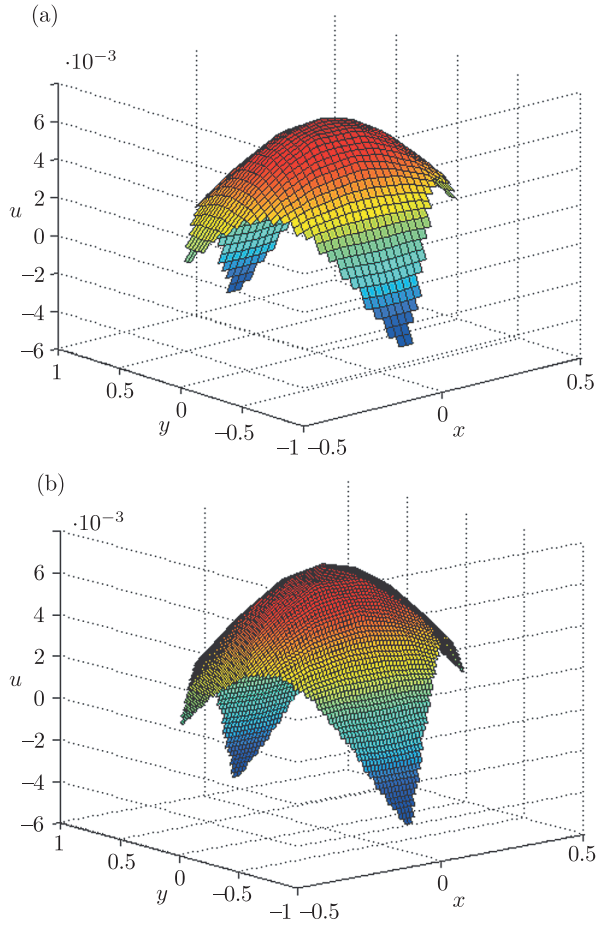

Figure 4. Concentration profiles interpolated from triangular into cartesian rectangular grid of different size

In the following example the results of calculations for a more irregular domain are shown. The shape of the domain is given by the parametric equations:

$$x(\theta) = 0.02\sqrt{5} + \big(0.5 + 0.2 \cdot \sin(5\theta)\big) \cdot \cos(\theta) \tag{8}$$

$$y(\theta) = 0.02\sqrt{5} + \big(0.5 + 0.2 \cdot \sin(5\theta)\big) \cdot \sin(\theta) \tag{9}$$

where $\theta \in [0, 2\pi]$.

Similarly to the previous example, the Dirichlet condition was set for each boundary. The analytical solution in time is given by Equation (10)

$$u = e^{-2t} \sin(x) \sin(y) \tag{10}$$

Figures 5(a)–(b) show the calculation domain described by Equations (8) and (9) with the triangular mesh of different sizes. It should be pointed out that the number of triangles increases in the region with a high radius of curvature. The increasing number of triangles leads to the increasing accuracy of the calculation in this area of the domain.

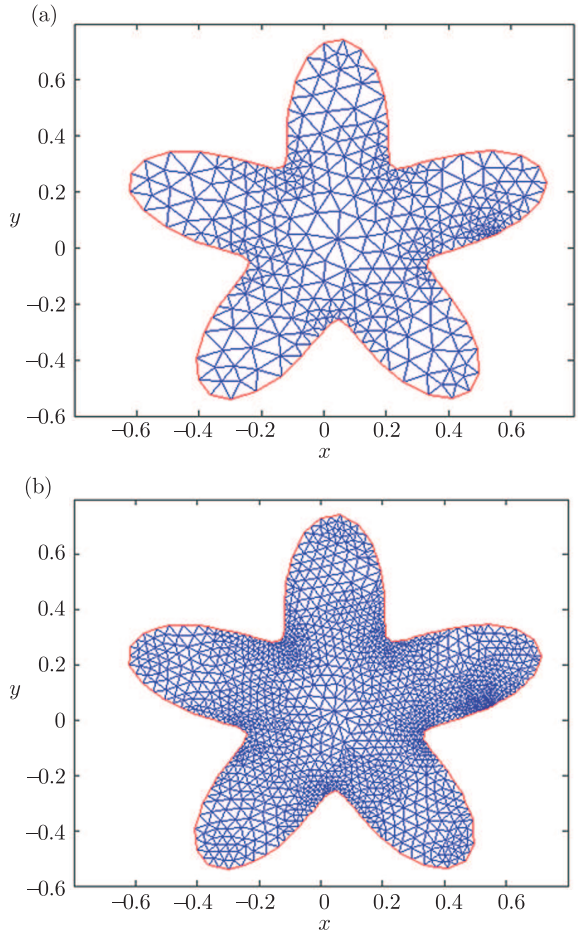

Figure 5. Calculation domain with triangular grid of different sizes

Tables 1 to 3 show the analysis of the solution for a different number of nodes in the triangle and regular mesh.

Table 1. Results of error calculations for different sizes of regular mesh. The number of elements in the triangular mesh is approximately $7 \cdot 10^2$

Number of nodes	L_1	L_2	$L_{\max}$
225×225	$3.49 \cdot 10^{-5}$	$7.09 \cdot 10^{-5}$	$3.17 \cdot 10^{-4}$
449×449	$3.47 \cdot 10^{-5}$	$7.08 \cdot 10^{-5}$	$3.17 \cdot 10^{-4}$

Table 2. Results of error calculations for different sizes of regular mesh. The number of elements in the triangular mesh is approximately $\sim 3 \cdot 10^3$

Number of nodes	L_1	L_2	$L_{\max}$
225×225	$8.47 \cdot 10^{-6}$	$1.71 \cdot 10^{-5}$	$1.02 \cdot 10^{-4}$
449×449	$8.40 \cdot 10^{-6}$	$1.70 \cdot 10^{-5}$	$1.02 \cdot 10^{-4}$

Table 3. Results of calculations for different sizes of regular mesh. The number of elements in the triangular mesh is approximately $\sim 10^4$

Number of nodes	L_1	L_2	$L_{\max}$
225×225	$2.09 \cdot 10^{-6}$	$4.19 \cdot 10^{-6}$	$3.14 \cdot 10^{-5}$
449×449	$2.05 \cdot 10^{-6}$	$4.13 \cdot 10^{-6}$	$3.11 \cdot 10^{-5}$

It can be seen that the precision of the calculation increases with the increasing number of triangle elements. However, the increasing number of elements in the regular mesh does not lead to any significant improvement. It means that the size of the triangular mesh determines the optimal size of the Cartesian grid.

Figures 6 and 7 show a comparison of the calculation results obtained with the use of our method with Euler and Crank-Nicholson standard techniques of solving differential equations. As can be seen the proposed method leads to high precision of calculation using a smaller number of nodes compared to standard techniques.

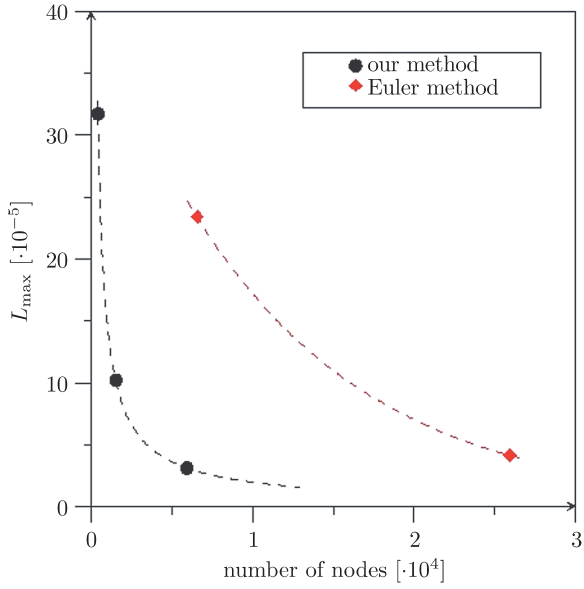

Figure 6. Results of error calculation of $L_{\max}$ for our method and Euler method

4. Conclusion

The Epitaxial Lateral Overgrowth method with the use of the Liquid Phase Epitaxy technique can be one of the promising techniques for future development of cost-efficient solar cells. Using the low cost and simple apparatus it is possible to produce high quality layers on low cost substrates. However, there are many technological parameters which have to be determined in order to obtain layers with an as high as possible aspect ratio. It requires numerous technological experiments. For this reason, numerical analysis seems to be a good solution as

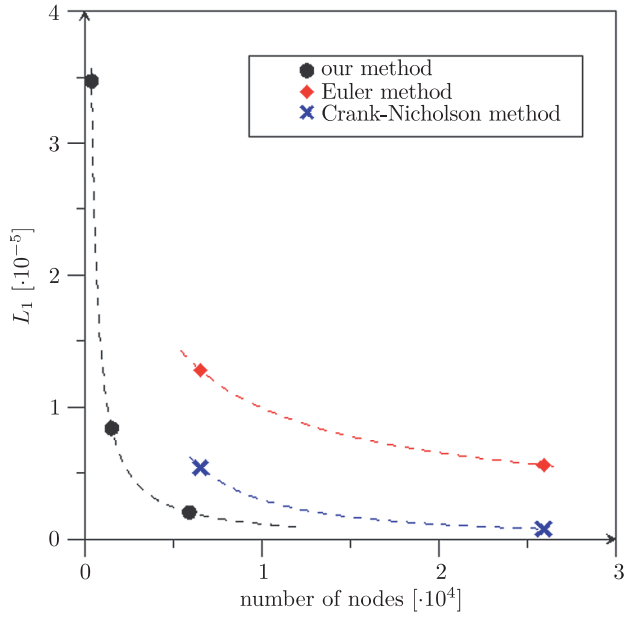

Figure 7. Comparison of efficiency of presented here method with Euler and Crank Nicholson techniques

it reduces the amount of experimental work and in consequence, the cost of the optimizing process. The developed computational model of the epitaxial growth requires high accuracy of concentration profile calculations especially near the moving interface. For this reason special modules implemented in the Matlab environment were created and verified in this paper. The results of the test show that the proposed solution works well and uses fewer computer resources than other numerical methods.

References

[1] Zytkiewicz Z R 2005 *Cryst. Res. Technol.* **40** (4/5) 321
[2] Zytkiewicz Z R 2002 *Thin Solid Films* **412** 64
[3] Nishinaga T 2002 *Journal of Crystal Growth* **237–239** 1410
[4] Jozwik I and Olchowik J M 2006 *Journal of Crystal Growth* **294** 367
[5] Liu Y C, Zytkiewicz Z R and Dost S 2005 *Journal of Crystal Growth* **275**, e953
[6] Yan Z, Naritsuka S and Nishinaga T 2000 *Journal of Crystal Growth* **209** 1
[7] Kimura M *et al.* 1996 *Journal of Crystal Growth* **167** 516
[8] Gulkowski S and Olchowik J M 2013 *Annual Set The Environment Protection* **15** 436
[9] Gulkowski S, Olchowik J M, Cieslak K and Moskvin P P 2012 *Materials Science – Poland* **30** (4) 414
[10] Gulkowski S, Olchowik J M and Cieslak K 2013 *Environmental Engineering IV* Pawłowski, Dudzińska & Pawłowski (eds), Taylor & Francis Group, London 457