

Numerical study of thermal stress during different stages of silicon Czochralski crystal growth

Amor Benmeddour and Salim Meziani

Laboratory of Mechanics, Faculty of Engineering Sciences,
Mentouri University, Road of Ain-El-Bey, Constantine, Algeria

(reçu le 20 Septembre 2009 – accepté le 25 Décembre 2009)

Abstract - In this paper, the influence of various crystal heights to the crystal/melt interface shape and thermal stresses distribution in the large diameter (300 mm) of the silicon single crystal growth in a Czochralski process was studied numerically. A two dimensional fluid flow and heat transfer with solidification model was developed. The Navier-Stokes and energy equations in melt and the heat conduction equation in crystal are solved using the control volume-based finite difference method. The thermal elastic stress fields for different stages are calculated from the temperature field by adopting the plane strain model in an axis-symmetric geometry of a cylindrical crystal. It was found that the melt/crystal interface shape becomes more concave and the maximum value of thermal stress in the crystal reduces as the crystal grows. A good agreement between our numerical simulations and those found in the literature is obtained.

Résumé - Dans cet article, l'effet de différentes longueurs du lingot de silicium sur la forme de l'interface solide / liquide et la répartition des contraintes thermiques dans des cristaux de silicium de large diamètre (300 mm) dans un système de croissance Czochralski a été étudiée numériquement. Un modèle bidimensionnel de l'écoulement du fluide et de transfert de chaleur avec solidification a été développé. Les équations de Navier-Stokes et d'énergie dans le liquide et l'équation de conduction de chaleur dans le cristal sont résolues par la méthode des volumes finis. La contrainte thermo élastique est calculée à partir du champ de température par l'adoption du modèle déformation plane dans une géométrie axisymétrique pour un cristal cylindrique. Les résultats obtenus montrent que la forme de l'interface solide / liquide devient très concave et la valeur maximum de la contrainte thermique dans le cristal diminue remarquablement pendant la croissance du lingot de silicium. Une bonne concordance entre nos résultats numériques et ceux trouvés dans la littérature est obtenue.

Keywords: Czochralski - Silicon - Solidification - Crystal/melt interface shape - Crystal height - Thermal stress.

1. INTRODUCTION

The Czochralski, 'CZ' crystal growth method illustrated in Figure 1-a, is one of the most important techniques for producing large size single crystals of silicon utilized in semiconductor devices or acousto-optic devices. In this process, a cylindrical crystal grows due to the phase change phenomena occurring in the melt and is then vertically pulled out of the system. The melt is placed in a cylindrical crucible, located in a furnace, and is heated above the melting temperature by a radiofrequency inductive heater.

In a CZ system, different types of heat transfer mechanism coexist in the growth setup. Heat transfer includes convection, conduction and radiation within the melt, conduction and radiation within the crystal and radiative heat exchange between exposed surfaces. However, it is hard to timely dissipate the enormous latent heat

induced by the solidification of Si melt when the crystal diameter is larger than 300 mm.

Consequently, temperature gradients tend to increase and inhomogeneous stress distribution is created [1, 2], and consequently contain a distinct region in the crystal with intensive multiplication of dislocations than smaller size crystals. Since thermal stresses and dislocations in electronic and optical materials reduce device performance and reliability, the reduction of dislocation densities and thermal stresses in large size crystals becomes an important issue. I

It was reported that during crystal growth process, there are compression stress in the core and tension stress in the periphery of the Si ingot [3]. The relation between the thermal stress and the dislocation density in a Si crystal has been verified [4, 5].

It is determined that controlling the thermal stress is one of the keys to grow dislocation free Si crystals [6]. In the later research by Takano [7] it was reported that with a larger crystal diameter the thermal stress affects the interface shape more significantly.

In this article, a fluid flow and heat transfer with solidification model was developed to simulate the temperature field and thermal stress distribution of 300 mm Si single crystal during the different stages of growth process and to reveal the effect of the crystal length on growing interface shape deflection and thermal stress.

2. MATHEMATICAL FORMULATION

2.1 Physical model and basic assumptions

The computational domain considered for the present analysis is shown in Figure 1-b. The process is a pseudo-steady state and axisymmetric with respect to the crystal pulling axis.

The melt flow is laminar and incompressible. Thermophysical properties of the melt are assumed to be constant. The crucible bottom is thermally insulated. The equilibrium solidification is considered at the crystal–melt interface and the crystallization front shape coincides with the melting temperature.

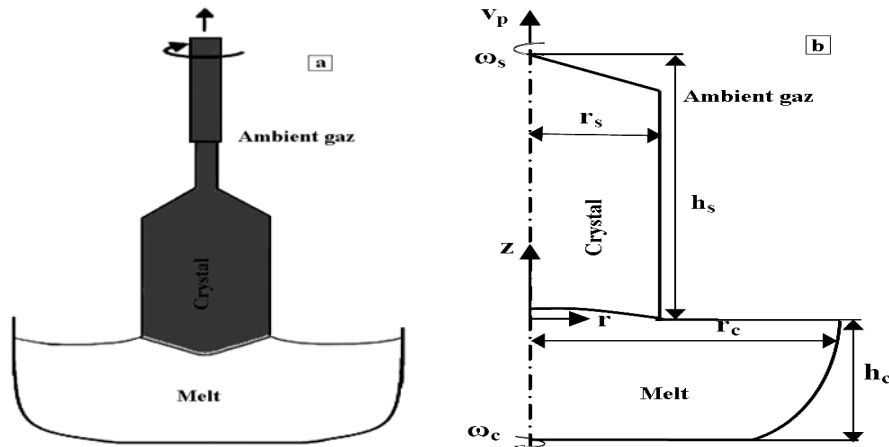


Fig. 1: a- Schematic diagram of the Czochralski growth, b- computational domain

The melt and the crystal are assumed to exchange radiation only with an ambient gas environment at a constant temperature, T_a . The geometry models and processing parameters are listed in **Table 1**.

Table 1: Geometrical and process parameters used for simulation

Crucible radius, r_c	200 mm
Crystal radius, r_s	150 mm
Crucible height, h_c	200 mm
Crystal height, h_s	150, 300, 450, 600 mm
Crystal rotational rate, ω_g	2 rpm
Crucible rotational rate, ω_c	0 rpm
Pulling rate, v_p	20 mm/h
Crucible wall temperature, T_c	1850 K
Ambient temperature, T_a	700 K

2.2 Mathematical model

The governing equations for the melt region are described by coupled Navier Stokes and energy equations with solidification. The Boussinesq approximation is used to account for buoyancy force in momentum equation via temperature dependence of density in gravity term.

Assuming axisymmetric conditions the partial differential equations governing steady-state, incompressible, and axisymmetric fluid flow are given in cylindrical coordinate as follows.

Continuity equation

$$\frac{\partial}{\partial z}(\rho u) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v) = 0 \quad (1)$$

Momentum equations

U-momentum

$$\frac{\partial}{\partial z}(\rho u u) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v u) = \frac{\partial}{\partial z} \left(\mu \frac{\partial u}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial u}{\partial r} \right) - \rho g \beta \nabla T - \frac{\partial p}{\partial z} \quad (2)$$

V-momentum

$$\frac{\partial}{\partial z}(\rho u v) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v v) = \frac{\partial}{\partial z} \left(\mu \frac{\partial v}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial v}{\partial r} \right) - \frac{\partial p}{\partial r} - \frac{\mu v}{r^2} + \frac{\rho w^2}{r} \quad (3)$$

W-momentum

$$\frac{\partial}{\partial z}(\rho u w) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v w) = \frac{\partial}{\partial z} \left(\mu \frac{\partial w}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial w}{\partial r} \right) - \frac{\mu w}{r^2} + \frac{\rho v w^2}{r} \quad (4)$$

Energy equation

$$\begin{aligned} \frac{\partial}{\partial z}(\rho u h) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v h) = \frac{\partial}{\partial z} \left(\frac{k}{C_p} \frac{\partial h}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{k}{C_p} \frac{\partial h}{\partial r} \right) \\ - \frac{1}{r} \frac{\partial}{\partial z}(\rho u \Delta H_f) - \frac{1}{r} \frac{\partial}{\partial z}(\rho r v \Delta H_f) \end{aligned} \quad (5)$$

where u , v and w are, the axial, radial and azimuthal components of the fluid flow velocity respectively, g the acceleration due to gravity, β the thermal expansion coefficient, h stands for the enthalpy, and the last two terms represent the convective source term solidification.

2.3 Boundary conditions

For the thermal boundary conditions, a constant temperature at the crucible walls and a convective-radiative heat transfer at gas-melt and gas-solid boundaries were employed.

For fluid flow, a no-slip boundary condition at the solid wall was considered. The boundary conditions corresponding to the surfaces given in Figure 1 for flow problem and temperature field are.

At the side and the top of the crystal

$$u = v_p, v = 0, w = r \cdot \omega_s, -k_s \frac{\partial T}{\partial r} = h(T - T_c) + \epsilon_s \sigma (T^4 - T_a^4) \quad (6)$$

At the melt/gas interface

$$u = 0, \frac{\partial v}{\partial z} = 0, \frac{\partial w}{\partial z} = 0, -k_m \frac{\partial T}{\partial r} = h(T - T_c) + \epsilon_m \sigma (T^4 - T_a^4) \quad (7)$$

At the side and bottom of the crucible

$$u = 0, v = 0, w = r \cdot \omega_c, T = T_c \quad (8)$$

At the centre line

$$\frac{\partial u}{\partial r} = 0, v = 0, w = 0, \frac{\partial T}{\partial r} = 0 \quad (9)$$

where k is the thermal conductivity, h is the heat exchange coefficient, ϵ is the emissivity of the material, σ is the Stefan–Boltzman constant, T_a is the outside temperature. ω_s and ω_c are the angular rotation rates of the crystal and crucible respectively.

3. NUMERICAL SOLUTION METHOD

The two dimensional differential equations (1)-(5) associated with the boundary conditions for the fluid flow and temperature field in the CZ configuration were solved numerically using a control volume-based finite difference method [8].

In order to couple the velocity field and pressure in the momentum equations, the SIMPLE-algorithm suggested by Patankar [9] was adopted. In order to account for the release of latent heat during solidification in the energy equation, a fixed grid enthalpy method advocated by Völler *et al.* [10, 11] was used in this work.

For the purpose of isothermal solidification modelling, an artificial thin mushy zone was assumed within which the latent heat of solidification was released. Based on the computed temperature field, the melting isotherm was predicted which corresponds to the position of crystal–melt interface.

The Von Mises stress was used, to express the thermal-elastic stress in the crystal, which was calculated after the temperature field in the crystal has been obtained by adopting the plan-strain model in axisymmetric geometry of a cylindrical crystal.

The calculation assumes that surface forces vanish on the surface of the crystal. The physical proprieties and the CZ growth conditions are given in **Table 2**.

Table 2: Physical and thermal properties of silicon

Property	Value	Unity
Melting temperature, T_m	1686	K
Latent Heat of fusion, ΔH_f	1110	kJ/kg
Thermal conductivity		
Solid, k_s	$(0.98)-(9.42 \times 10^{-4}) \cdot T$	W/K.m
Liquid, k_m	66.5	“
Specific Heat		J/K.kg
Solid, C_{p_s}	1000	“
Liquid, C_{p_m}	915	“
Density		kg/m ³
Solid, ρ_s	2530	“
Liquid, ρ_m	2570	“
Emissivity		
Solid, ε_s	$(0.9)-(26 \times 10^{-5}) \cdot T$	
Liquid, ε_m	0.30	
Heat exchange coefficient, h	7	W/m ² .K
Thermal expansion Coefficient, β	3.2×10^{-6}	1/K
Poisson's ratio	0.25	
Young's modulus, E	1.31×10^{11}	Pa

4. RESULTS AND DISCUSSION

In this section, a series of numerical simulations has been conducted to calculate the temperature field in the crystal, stress field due to thermal expansion and the impact of the crystal heights on growing interface shape deflection and thermal stress are discussed.

Fig. 2 shows the simulation results of temperature fields in the melt and crystal, and the corresponding thermal-elastic stress distribution in the crystal for the different growth stages.

When $v_p = 10$ mm/h, and the height of the crystal is about (a) 150 mm, (b) 300 mm, (c) 450 mm and (d) 600 mm. In these figures, the left side shows the isotherms in the melt and crystal separated by steps of 30 K.

The right side shows the iso-stress curves in the crystal separated by steps of 3 MPa.

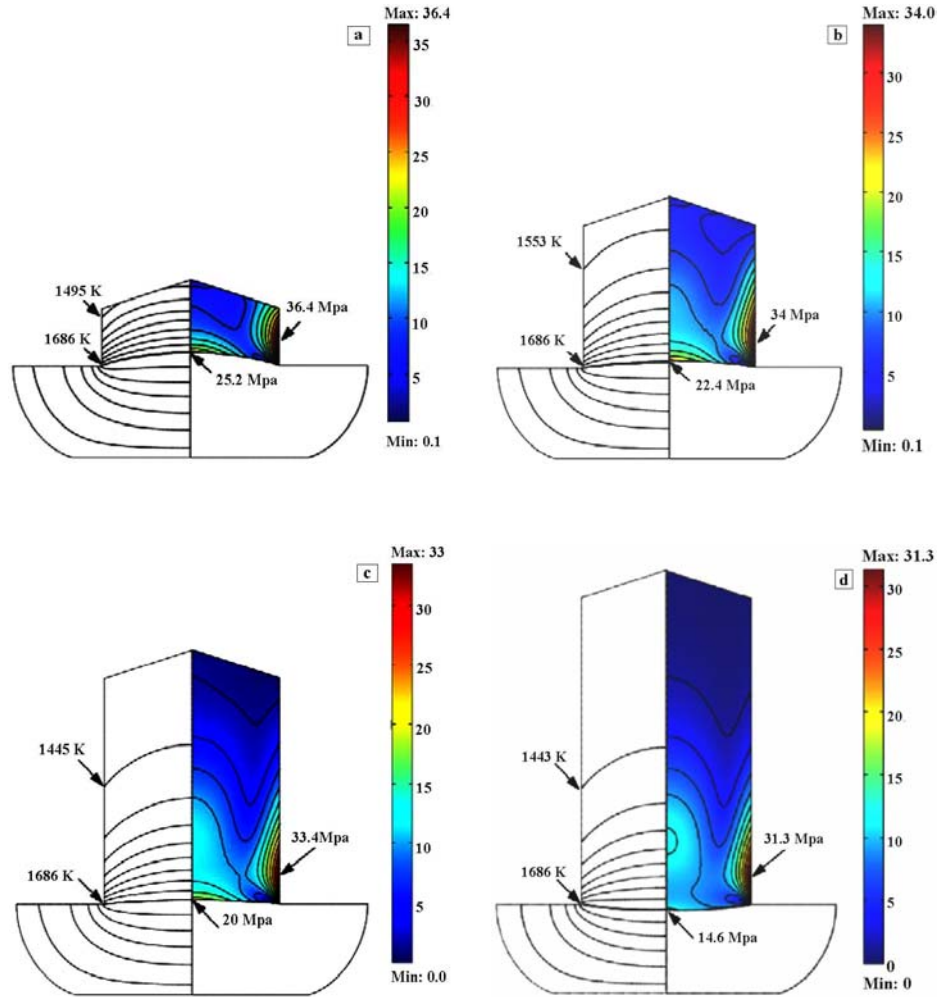


Fig. 2: Temperature and thermal stress distribution for different heights of the crystal

For all results represented in Fig. 2, we can observe a remarkable phenomenon, two hot spots corresponding with two maxima of stress for various lengths, one in the center of the melt/crystal interface and the other at the edge of the crystal.

The maximum thermal stress at crystal edge is larger than at the crystal/melt interface and the interface shape is significantly affected during growth.

Fig. 3 shows the evolution of crystal/melt interface deflection at different heights. The growing interface shape changes from convex to concave with increasing the length. When the length is low (150 mm), the interface is more convex. As the length become larger, the interfaces become concave to the crystal.

The maximum deflection of the growth interface will increase from 22.5 to -10 mm as varying the length from 150 to 600 mm since the pulling rate kept constant.

This change of interface shape affects the variation of the von Mises stress along the interface, as shown in Fig. 4. We can observe that the thermal stress profiles go from a W-shape to a U-shape and the maximum thermal stress located at the center of the interface is the highest (25.2 MPa) in the first case when the interface is convex.

As the interface shape changes, the stress becomes much smaller at the center (14.6 MPa), but the stress at the edge of the interface becomes larger.

It is now obvious that the melt/crystal interface shape has a strong effect on the maximum thermal stress in the growing Si crystal, the value of the von Mises stress gets larger in the case where the interface become more convex to the crystal, this is consistent qualitatively with our result [12].

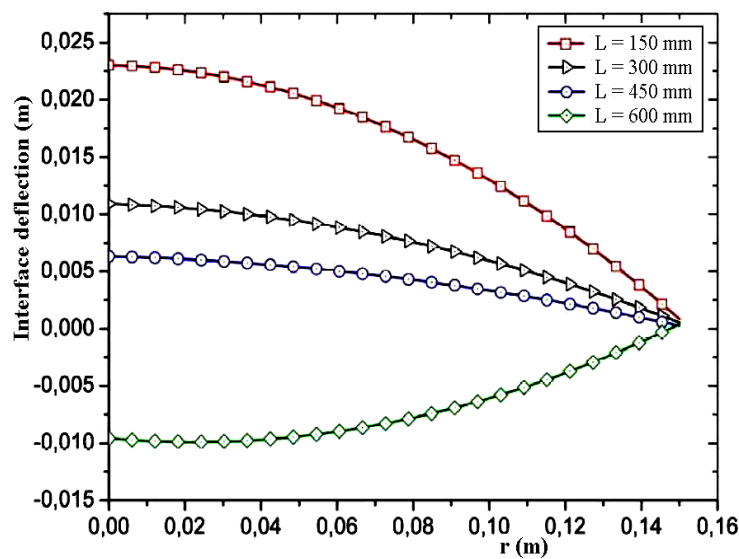


Fig. 3: The crystal/melt interface deflection at different heights

The von Mises stress invariant along the edge of the crystal for different crystal growth heights are shown in Fig. 5. We can observe at first, that increasing the length induces a decreasing stress level, but the variation of stress is not significantly.

The peak values of the stress at the edge of crystal increase from 36.4 MPa to 31.3 MPa, as the length change from 150 mm to 600 mm. This is mainly due to the increasing crystal grows longer.

The decrease in stress can be explained by heat transfer mechanisms inside the crystal. The temperature gradient is dependent on surface area.

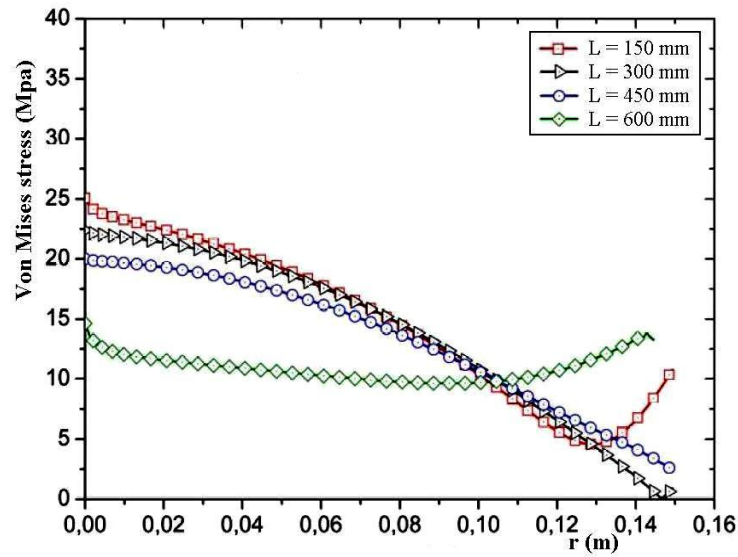


Fig. 4: Von Mises stress along the interface for different crystal growth heights

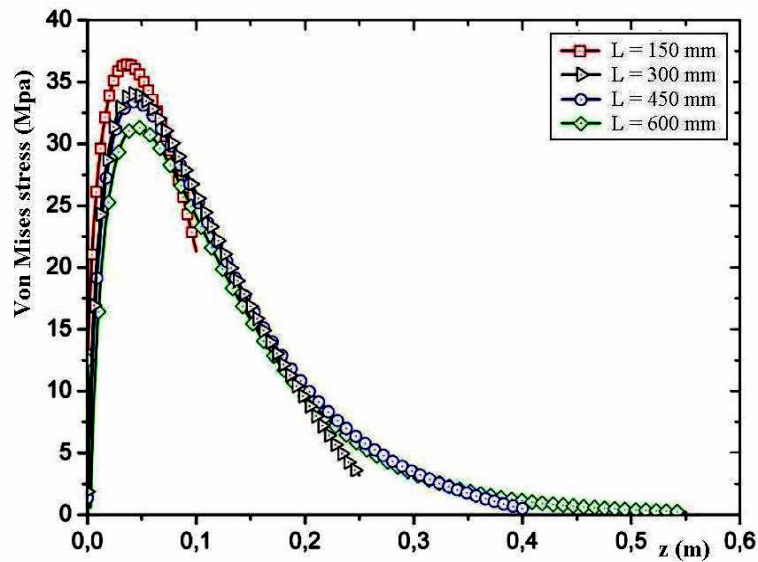


Fig. 5: Von Mises stress along the edge for different crystal growth heights

The crystal exchanges more heat with the outside environment, resulting in isotherm curvature. Small temperature gradients can exist in the crystal and stress increase when the crystal length is large.

In addition, the crystal exchanges less heat by radiation with the outside environment and its vertical temperature gradient decreases and stress decrease when the length is low.

Secondly, the location where the maximum stress appears does not change with the growth. This prediction of stress variation as the crystal grows is in complete agreement with the observation of Volkl *et al.* [13].

The maximum value of the Von Mises stress obtained in the present calculation are slightly larger than those given by Muzinek *et al.* [6], so it is very dangerous and the dislocation may be generate at the growing interface.

5. CONCLUSION

We have been studied numerically, the temperature field and thermal stress distribution of Silicon single crystal during the different stages of growth process.

The model predicts the location of two maximum stress spots, at the edge of the crystal and at the crystal/melt interface center. The thermal stress at the edge is larger than at the interface center.

As the crystal grows, the locations where the maximum stress appears does not change, but the value of the peak stress decreases with the crystal height. The mechanism of this reduction in the maximum stress with crystal height can be attributed to a decreased radial temperature gradient.

The results indicate that the interface shape is significantly affected during growth, when the crystal height is low, the interface is more convex and the thermal stress is highest.

With increasing the growth height, the interface shape convents from convex to concave and the maximum value of thermal stress in the crystal decreases rather remarkably. Finally, we wish to mention the excellent agreement between our numerical results and those given in the literature.

NOMENCLATURE

u, v, w : Velocities- axial, radial and azimuthal, m/s	ω_s : Crystal rotational rate, rad/s
r, z : Polar coordinates, m	ω_c : Crucible rotational rate, rad/s
p : Pressure; Pa	v_p : Pulling rate, m/s
g : Acceleration due to gravity, m/s ²	ΔH_f : Latent Heat of fusion, J/kg
	C_p : Specific heat, J/K.kg
T_c : Crucible wall temperature, K	ρ_s : Density of solid, kg/m ³
T_m : Melting temperature, K	ρ_m : Density of melt, kg/m ³
T_a : Ambient temperature, K	σ : Stefan-Boltzman constant,
r_c : Crucible radius, m	ϵ_m : Melt emissivity
r_s : Crystal radius, m	ϵ_s : Crystal emissivity
h_m : Melt heat exchange coefficient, W/m ² .K	h_s : Crystal heat exchange coefficient, W/m ² .K
h_c : Crucible height, m	h_s : Crystal length, m
k_s : Crystal thermal conductivity, W/mK	E : Young's modulus, Pa

k_m : Melt thermal conductivity, W/mK

μ : Viscosity

B : Thermal expansion

β : Poisson's ratio

REFERENCES

- [1] N. Miyazaki, H. Uchida, T. Munakata, K. Fujioka and Y. Sugino, 'Thermal Stress Analysis of Silicon Bulk Single Crystal during Czochralski Growth', Journal of Crystal Growth, Vol. 125, N°1-2, pp. 102 – 111, 1992.
- [2] N. Miyazaki, 'Development of a Thermal Stress Analysis System for Anisotropic Single Crystal Growth', Journal of Crystal Growth, Vol. 236, N°1-3, pp. 455 – 465, 2002.
- [3] T. Tsukada, M. Hozawa and N. Imaishi, 'Effect of a Radiation Shield on Thermal Stress Field during Czochralski Crystal Growth of Silicon', Journal of Chemical Engineering of Japan, Vol. 23, N°2, pp. 186 - 191, 1990.
- [4] A.S. Jordan, R. Caruso and A.R. von Neida, 'A Thermoelastic Analysis of Dislocation Generation in Pulled GaAs Crystal', Bell. Syst. Tech. J, Vol. 59, 593, 2002.
- [5] A.S. Jordan, A.R. von Neida and R. Caruso, 'A Comparative Study of Thermal Stress Induced Dislocation Generation in Pulled GaAs, InP and Si Crystals', Journal of Applied Physics, Vol. 52, N°5, pp. 3331 – 3336, 1981.
- [6] A. Muiznieks, G. Raming, A. Muhlbauer, J. Virbulis, B. Hanna and W.V. Ammon, 'Stress-Induced Dislocation Generation in Large FZ- And CZ-Silicon Single Crystals Numerical Model and Qualitative Considerations', Journal of Crystal Growth, Vol. 230, N°1-2, pp. 305 – 313, 2001.
- [7] K. Takano, Y. Shiraishi, J. Matsubara, T. Iida, N. Takase, N. Machida, M. Kuramoto and H. Yamagishi, 'Global Simulation of the CZ Silicon Crystal Growth up to 400 mm in Diameter'. Journal of Crystal Growth, Vol. 229, N°1, pp. 26 – 30, 2001.
- [8] P. Sabhapathy and M.E. Salcedan, 'Numerical Analysis of Heat Transfer in LEC Growth of GaAs', Journal of Crystal Growth, Vol. 97, N°1, pp. 125 – 135, 1989,
- [9] S.V. Patankar, 'Numerical Heat Transfer and Fluid Flow', Hemisphere, Washington DC, 1980.
- [10] V.R. Völler and C. Prakash, 'A Fixed-Grid Numerical Modelling Methodology for Convection-Diffusion Mushy Region Phase Change Problems', International Journal Heat Mass Transfer, Vol. 30, N°10, pp. 1709 – 1720, 1987.
- [11] W.D. Bennon and F.P. Incropera, 'A Continuum Model for Momentum, Heat and Species Transport in Binary Solid-Liquid Phase Change Systems, I: Model Formulation', International Journal Heat Mass Transfer, Vol. 30, N°10, pp. 2161 – 2170, 1987.
- [12] A. Benmeddour and S. Meziani, 'The Effect of Pulling Rates on the Interface Shape and Thermal Stress in the Si Single Crystal Growth by Czochralski Method', International Review of Mechanical Engineering, Vol. 3, N°3, pp. 353 – 357, 2009.
- [13] J. Volkl and G. Muller, 'A New Model for the Calculation of Dislocation Formation in Semiconductor Melt Growth by Taking into Account the Dynamics of Plastic Deformation', Journal of Crystal Growth, Vol. 97, N°1, pp. 136 – 145, 1989.