

Finite Element Simulation of the Liquid Silicon Oriented Crystallization in a Graphite Mold

Alexey I. Borovkov

Vadim I. Suprun

Computational Mechanics Laboratory, St. Petersburg State Technical University,
Russia

Abstract

The mathematical model of the liquid silicon oriented crystallization in the graphite mold is presented. During the simulation of the coupled (semi-coupled) thermoelasticity problem the transient temperature field, stresses and strain in a casting and a graphite mold at phase change and subsequent cooling are calculated. The plastic strains are also determined. In mathematical model the increase of silicon volume (8%) and discontinuous variations of the thermal and mechanical properties at phase change are taken into account. The program module based on APDL is created for conducting subsequent coupled analyses. It is used to perform the transient structural analysis.

Introduction

The development of many branches of industry is closely connected with the development of technologies and high-purity material manufacture. Semi-conductor silicon, on the base of which about 98% of all semi-conductor appliances are manufactured, takes its distinctive place among high-purity materials. No branch of modern industry develops so fast as semi-conductor electronics, which success is indissolubly associated with achievements in the semi-conductor material technology.

The development of new fields of science and technology, in particular – power information optics, urgent necessity of significant decrease of costs of solar energy semi-conductor converters stimulate the development of new courses of obtaining parts based on semi-conductor purity silicon. The necessity of the industrial using of laser material-treatment technologies put forward the problem of creating moderate-power laser set reflectors. In choosing a reflector-material the following requirements are advanced to the foreground: its accessibility, technological effectiveness in manufacture, operational dependability, production costs. All these requirements are completely met by reflectors if high-purity semi-conductor silicon is used as their structural material. The choice of semi-conductor silicon for manufacture of power optics reflectors is caused by its low specific weight, high hardness, crystal lattice perfection, low linear coefficient of thermal expansion, high modulus of elasticity and satisfactory thermal conductivity.

At present, semi-conductor purity silicon crystals applicable for using in optical instrument production may be manufactured at industrial scale either by the Chokhralsky's method or by the casting method. The Chokhralsky's method makes it possible to obtain large silicon crystals; however their diameter is restricted by the diameter of the used crucible and does not exceed 220..250mm at present. For obtaining larger-sized silicon monocrystals, the casting method is generally used. At present, for casting process implementation it has been specially designed and manufactured a pilot-plant set for casting silicon articles. Various construction of casting molds for producing articles of different function have also been developed.

The goal of this work is the finite element modeling (FEM) of silicon plate oriented crystallization in the graphite mold.

Axisymmetrical Statement of the Problem

In the FEM process we will consider a simplified model of the actual physical process. For further computations, let us make the following assumptions:

- All silicon amount at the initial time instant is present in a graphite mold in liquid state.

- The temperature inside a silicon mold at the initial time instant is uniform and higher than the silicon crystallization temperature.
- The temperature inside a silicon mold at the initial time instant is uniform and considerably lower than the silicon crystallization temperature.
- The contact in the casting-mold interface is ideal, i.e. the conditions of equal temperature and continuity of the displacement vector and the stress vector are fulfilled in the casting-mold interface.

This statement of the problem does not take into account the complex process of filling a mold with a melt, which, in general, is not axisymmetric. Thus, the fact that when all the melt is poured into a mold, crystallization of some amount of silicon has already taken place inside it, and there is a great temperature gradient, which, in its turn, induces the complex stress-strain state of a casting.

Material Properties

In further computations we will suppose that silicon density diminishes spasmodically during crystallization from 2490kg/m^3 in a liquid phase to 2330 kg/m^3 in a solid phase and remains constant with further temperature lowering (See Figure 1.) Dependence of silicon thermal conductivity on temperature is shown in Figure 2. Young's modulus for silicon $E=130\text{GPa}$ and Poisson's ratio $\nu=0.28$ in solid phase are assumed to be independent from temperature. A volume change in the process of crystallization is taken 8%, melting temperature – $1414\text{ }^\circ\text{C}$.

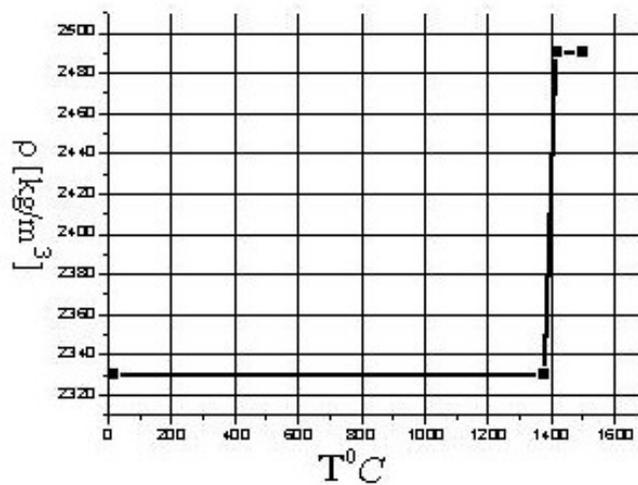


Figure 1 - Mat. Density

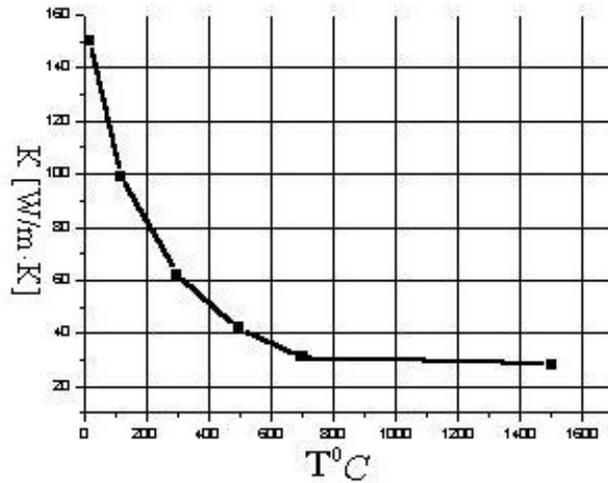


Figure 2 - Mat. conductivity

Phase Change

Every phase change is accompanied by spasmodic variations of some values characterizing material properties. Specific thermodynamic potential $\varphi(T, P)$ remains continuous at any transitions; however its derivatives may undergo breaks. A phase change when first derivatives vary spasmodically is called first-type phase change. A phase change when first derivatives remain continuous, but second derivatives vary spasmodically is called second-type phase change.

Let us consider the first-type phase change. As

$$s = \left(\frac{\partial \varphi}{\partial T} \right)_p ; \quad v = \left(\frac{\partial \varphi}{\partial P} \right)_T ;$$

then this change is characterized by spasmodic variation of specific entropy or specific volume or of both these parameters combined. Spasmodic variation of specific entropy means that phase change is accompanied by heat emanation or absorption. Heat amount necessary to be conveyed to a matter mass unit in order to transfer it quasi-statically from state 1 to state 2 is determined by the following equation:

$$q = T(s_2 - s_1).$$

All variations of the state of aggregation of matter are accompanied by heat emanation or absorption and a volume change; therefore they are related to the first-type phase change.

Silicon transforms from liquid into solid at melting temperature $T=1414$ °C. Latent heat is emanated during the process of solidification. For taking latent heat into account, it is necessary to assume the temperature range defining a phase change zone. Inside this zone spasmodic variation of some physicomaterial properties of crystallizing matter (density, thermal capacity etc.) takes place. For this particular state of the problem, it is suggested the following temperature range of the phase transition zone: $T=[1380..1420]$ °C.

Dependence of silicon enthalpy on temperature is presented in Figure 3. Variation of the curve slope on the graph in the phase transition zone is caused by emanation of latent heat.

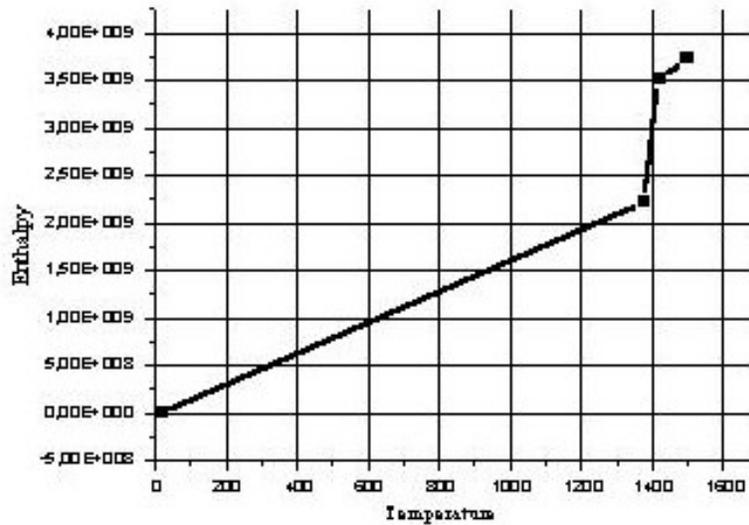


Figure 3 - Mat. enthalpy

FE Model and Analysis Procedure

Some parameters of FEM:

- Applied finite element: plane 4-node element PLANE55 – for solution of the nonstationary thermal conductivity problem;
plane 4-node element PLANE42 – for solution of the elastoplasticity problem.
- Number of elements: 3528
- Number of nodes: 3673
- Number of degrees of freedom: 3673 – for solution of the problem of nonstationary thermal conductivity;
7346 – for solution of the elastoplasticity problem.

The problem of thermoelastoplasticity is solved in the semi-coupled statement, i.e. at first, the problem of thermal conductivity is solved, and then, after obtaining transient temperature distribution fields, the stress tensor component distribution and the plastic strain field are determined (successive analysis).

A phase change is modeled by assumption of material enthalpy as a function of temperature. The spasmodic increase of volume at a phase change is modeled by the appropriate increase of linear coefficient of thermal expansion in the phase change zone. Conveyance of the transient temperature field taken from the solved problem of conductivity to the problem of thermoelastoplasticity is implemented with use of the software compiled in APDL Lang.

Transient Thermal Analysis

As it was mentioned above, the problem of thermo-conductivity is solved in the axisymmetrical statement. A half of the cross-section of a casting mold, with liquid silicon inside it, is presented in Figure 4 (all dimensions are in millimeters).

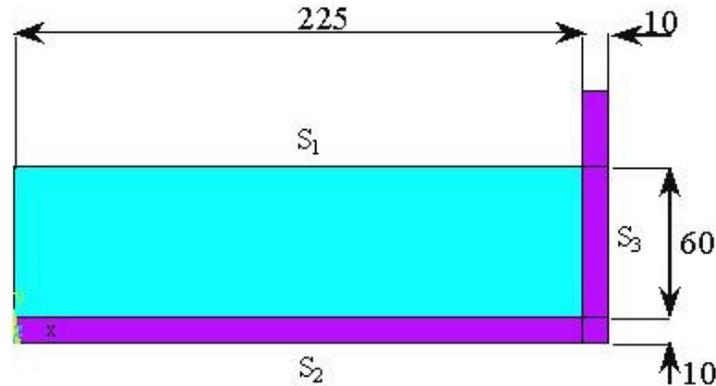


Figure 4 - Cross-section of a casting mold

Initial and Boundary Conditions

It is assumed that at the initial time instant silicon temperature is constant and equal to $T_{sil}|_{t=0} = 1500^{\circ}C$.

Let the graphite mold at the initial time instant be at the temperature $T_{gr}|_{t=0} = 1000^{\circ}C$.

The upper surface of a silicon casting is heat-isolated $\nabla T|_{s_1} = 0$

The following boundary conditions of the second type are given on the surface of the graphite mold:

$$-k\underline{n} \cdot \nabla T|_{s_2} = 20000 \frac{J}{m^2 \cdot s}$$

$$-k\underline{n} \cdot \nabla T|_{s_3} = 5000 \frac{J}{m^2 \cdot s}$$

Results and discussion

In the FEM process the time interval up to 4800 s was analyzed.

Research of Crystallization Front Movement

Locations of the phase change zone at different time instances are presented in Figures 5-8. A liquid phase change zone is depicted by red color, a formed monocrystal zone – by blue color. Between these two zones a phase change zone, marked by green color, is disposed.



Figure 5 - Phase change zone at $t=30\text{s}$

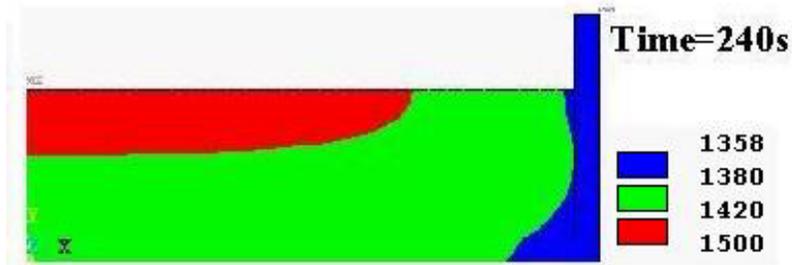


Figure 6 - Phase change zone at $t=240\text{s}$

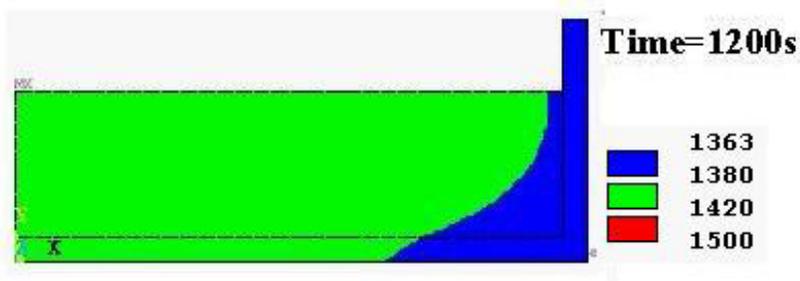


Figure 7 - Phase change zone at $t=1200\text{s}$



Figure 8 - Phase change zone at $t=2850\text{s}$

Determination of Temperature Field

The diagrams of temperature distribution at different time instances ($t=30, 1800, 3000, 4800$ s) are presented in Figures 9-12.

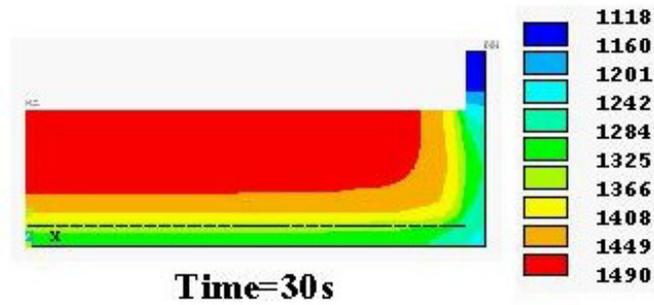


Figure 9 - Temperature distribution at $t=30$ s

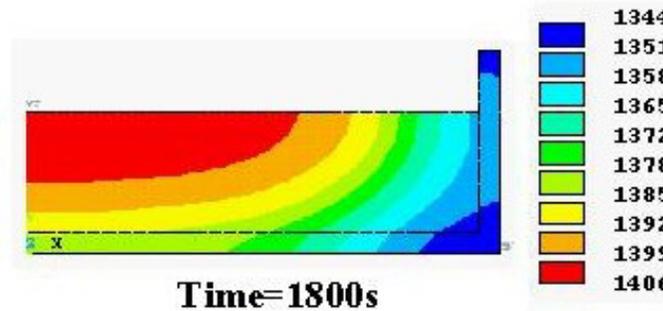


Figure 10 - Temperature distribution at $t=1800$ s

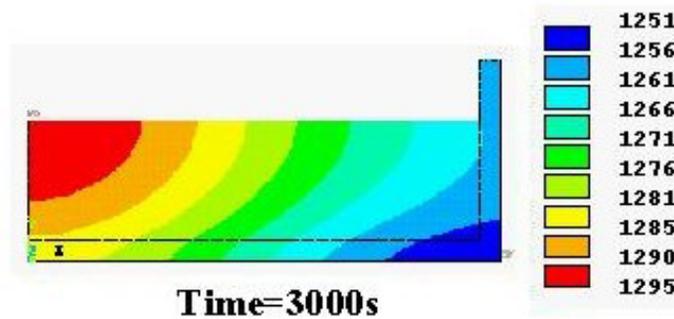


Figure 11 Temperature distribution at $t=3000$ s

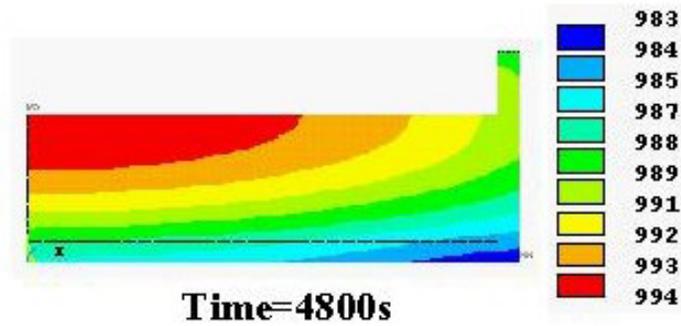


Figure 12 - Temperature distribution at t=4800s

As it is seen from obtained temperature fields, at the initial stage of crystallization a significant temperature gradient originates in the mold-casting interface zone, owing to large difference between original temperatures of liquid silicon and a graphite mold (See Figure 9). Then, in the process of silicon crystallization, temperature gradient inside the system “silicon-graphite mold” decreases, and when all silicon is in a solid state, a temperature drop in a casting does not exceed 45°C (See Figure 11). After the end of the crystallization process, the combined cooling of a casting and a mold takes place, and at the instant $t=4800s$ the difference between maximal and minimal temperatures comes down to 11°C (See Figure 12).

Investigation of Temperature Dependence on Time at Different Points of a Casting

The points inside a casting marked in Figure 13 are those, for which the graphs of temperature dependence on time are built (See Figure 14). At first, matter crystallization takes place at points 1 and 4, then – at point 2, and the last portion of matter transforms into a solid phase at point 3.

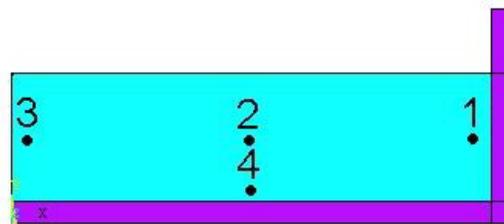


Figure 13 - Points inside a casting

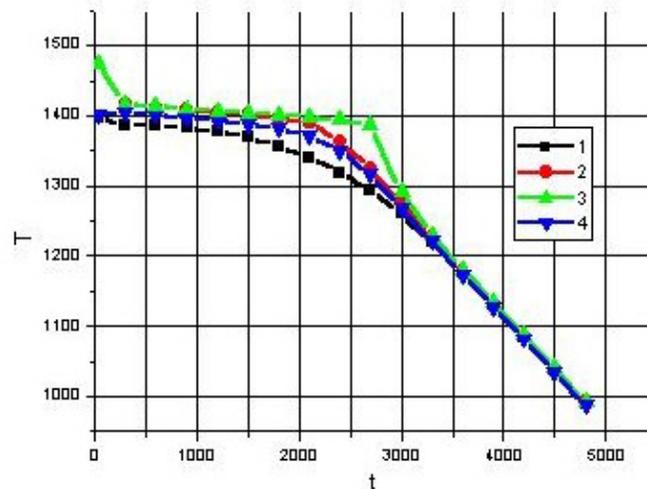


Figure 14 – Temperature dependence on time

When temperature in the points reaches the upper boundary of the phase change zone, the crystallization process originates. The start of crystallization corresponds to the beginning of a horizontal line in the graph. Then the process ceases, temperature insignificantly changes during some period of time, being in the range of the phase change zone (horizontal parts of graphs). Insignificant temperature variations during sufficiently large time interval may be explained by that the heat transferred by a liquid phase into a mold through a solidified part of matter is compensated by emanation of latent heat at phase change. After the process of silicon crystallization is finished, temperature decreases sufficiently fast (the cooling process proceeds at approximately the same velocity in various points of a casting).

Solution of the Problem of Anisothermal Elasto-Plastic Behavior of Material

It is required to find a stress-strain state of a casting and a mold at various time instances using the obtained transient temperature field. Also, it is required to determine the field of plastic strains emerging in a silicon casting in the process of crystallization and subsequent cooling.

Boundary Conditions

Let us suppose that a mold is put on the horizontal surface, i.e. the normal component of the displacement vector on the lower mold surface is equal to zero $u_n|_{s_2} = 0$.

Mathematical Model

In the process of the silicon crystallization FE simulation, it is necessary to take into account the 8% - increase of specific volume of silicon at a phase change.

Let us consider an infinitely minor parallelepiped with ribs dx , dy , dz parallel to principle axis of the strain tensor; its volume before deformations is $dV = dx dy dz$ and after deformation –

$$d\tilde{V} = dx dy dz (1 + \varepsilon_1)(1 + \varepsilon_2)(1 + \varepsilon_3).$$

Relative change of the volume, called volume expansion, is equal to

$$\mathcal{G} = \frac{d\tilde{V} - dV}{dV} = (1 + \varepsilon_1)(1 + \varepsilon_2)(1 + \varepsilon_3) - 1.$$

From the previous equation, assuming principle strains equal to each other, i.e. $\varepsilon_1 = \varepsilon_2 = \varepsilon_3$, and taking \mathcal{G} equal to 0.08 (8%), we find linear strain, which comes to $\bar{\varepsilon} = 0.026$. Then from the equation

linking linear strain with temperature variation $\bar{\varepsilon} = \int_{T'}^{T''} \tilde{\alpha} dT$, we find linear coefficient of thermal

expansion $\tilde{\alpha}$ conforming to the given linear strain at $T' = 1380^{\circ}C$ and $T'' = 1420^{\circ}C$. Dependence of α on temperature is shown in Figure 15. For the temperature range of phase change ($T=1380..1420^{\circ}C$) it is equal to $\alpha = \tilde{\alpha} = -6.57 \cdot 10^{-4}$.

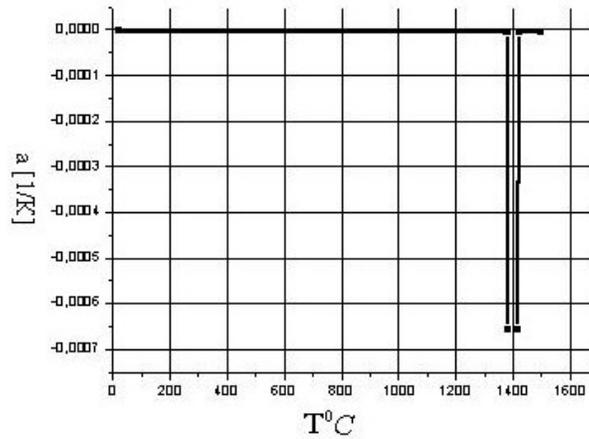


Figure 15 - Dependence of α on temperature

In the solution of the problem, the variant of dependence of Young's modulus on temperature presented in Figure 16 is suggested to be considered. Young's modulus in the phase change zone varies linearly, from Young's modulus for a liquid phase equal to $E_l = 1 \cdot 10^{11} Pa$ to that for solid phase equal to

$$E_s = 1.3 \cdot 10^{11} Pa.$$

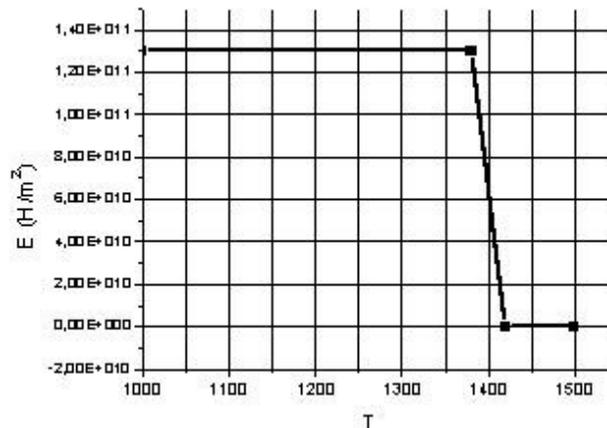


Figure 16 - Mat. Young's modulus

Let us suppose in further computations that both a casting and a mold undergo deformation as a single. This means that the condition of continuity of the displacement vector and the stress vector are fulfilled, i.e.:

$$[\underline{u}] = 0, \quad [\underline{n} \cdot \underline{\sigma}] = 0,$$

where $[\underline{u}] = \underline{u}^+ - \underline{u}^-$ - difference between displacement vectors in a casting and in a mold at their interface; $[\underline{n} \cdot \underline{\sigma}] = \underline{n} \cdot \underline{\sigma}^+ - \underline{n} \cdot \underline{\sigma}^-$ - difference between stress vectors on the casting-mold interface.

It should be mentioned that stresses presented in diagrams of stress were computed in Pascals, and under condition of linear variation of Young's modulus in the phase change zone (See Figure 15).

Results and discussion

Distributions of Stress Tensor Components and Von Mises Equivalent Stresses

Time instant $t=2400$ s conforms to the moment when all the stress tensor components come to the stationary level. This means that during subsequent cooling of a casting and a mold the stress values change insignificantly.

The diagrams of von Mises Equivalent Stress distributions at different time instances are presented in Figures 17-21. The results obtained expose that maximal equivalent stresses appear in the central zone of a casting, on crystal surfaces and in the place of contact of a casting with the bottom of a casting mold. Minimal equivalent stresses emerge inside the mold body.

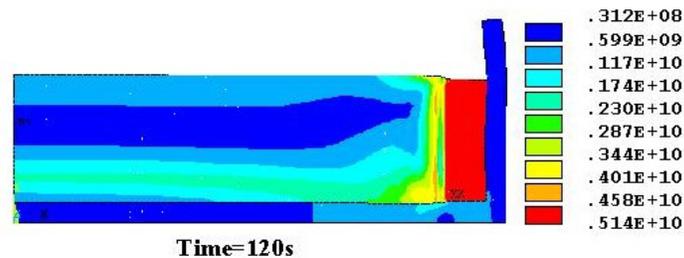


Figure 17 - Von Mises Stress at t=120s

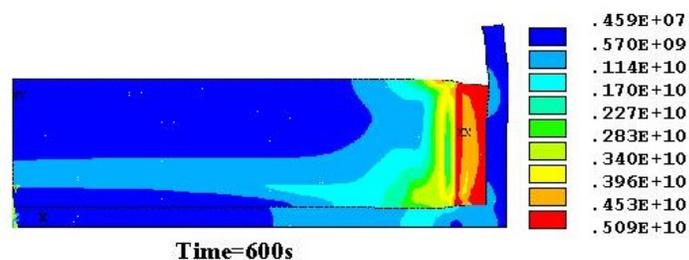


Figure 18 - Von Mises Stress at t=600s

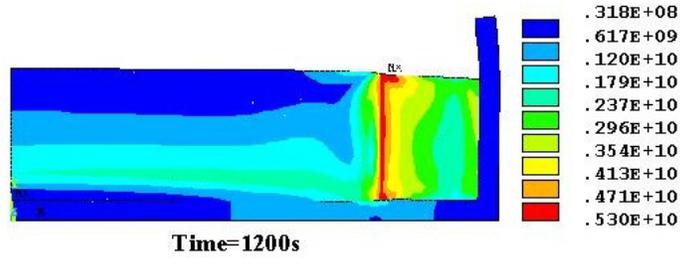


Figure 19 - Von Mises Stress at t=1200s

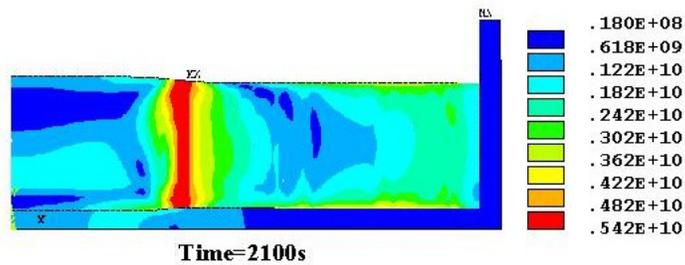


Figure 20 - Von Mises Stress at t=2100s

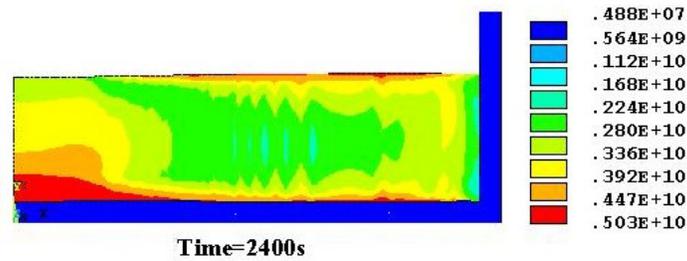


Figure 21 - Von Mises Stress at t=2400s

Plastic Strain Field

The diagram of distribution of plastic strains originating in a casting at a phase change are presented in Figures 22-24. During silicon crystallization, in the range of a phase change emerges a zone of large equivalent stresses, which exceed yield strength. In consequence of it, silicon undergoes plastic deformation during solidification.

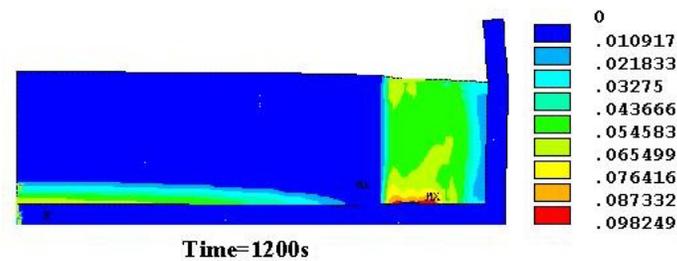


Figure 22 - Plastic Strain at t=1200s

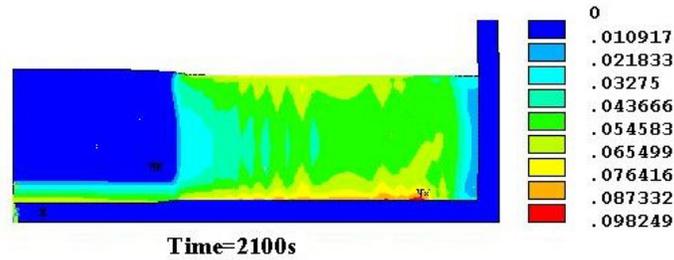


Figure 23 - Plastic Strain at t=2100s

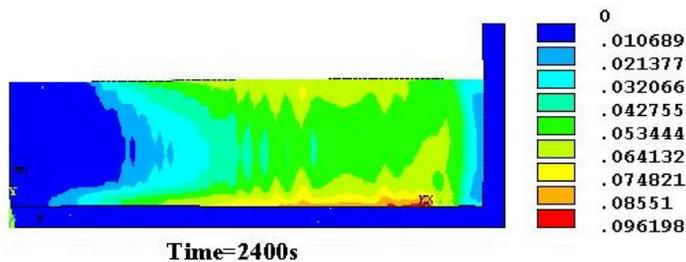


Figure 24 - Plastic Strain at t=2400s

Stress Dependence on Coordinates in the Cross-Section of a Casting and a Mold

There were built graphs of stress dependence on coordinates in the chosen cross-section AA (See Figure 25) of a casting and a mold at various time instances. In the graph (See Figures 26-29) one may watch variation in time of stress distribution inside a casting and a mold. It is seen that vertical and circumferential stresses undergo spasmodic variation at the phase change range. Radial stresses also vary during crystallization, however, they are significantly lesser than vertical ones (especially at the initial stage of the crystallization process).



Figure 25 - Cross-section AA

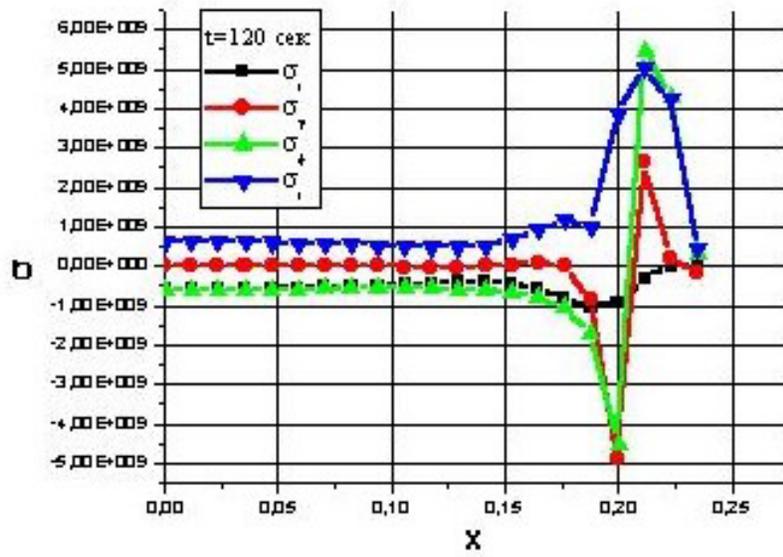


Figure 26 - Stress Dependence on Coordinates at t=120

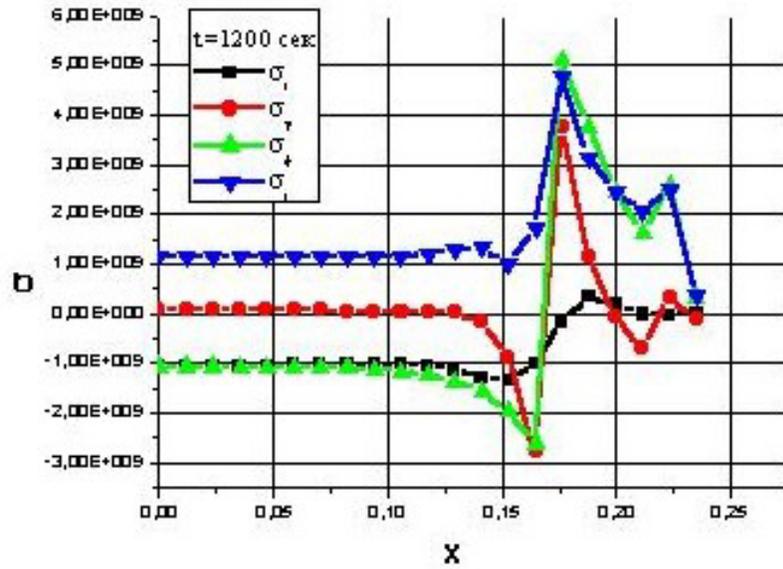


Figure 27 - Stress Dependence on Coordinates at t=1200

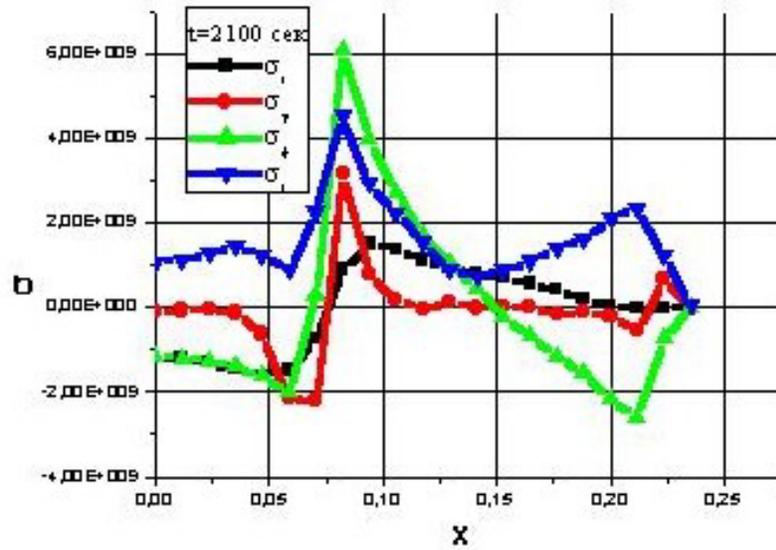


Figure 28 - Stress Dependence on Coordinates at t=2100

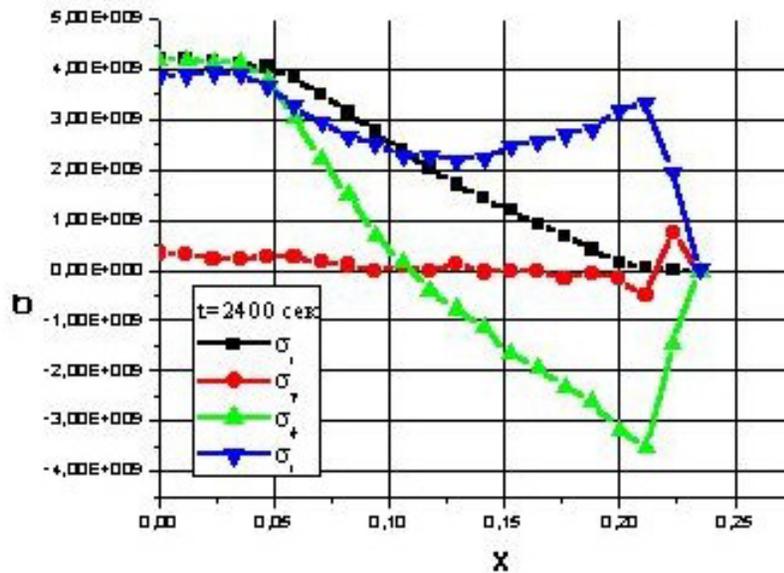


Figure 29 - Stress Dependence on Coordinates at t=2400

Stress Dependence on Time at Chosen Point of a Casting

Stress dependence on time at point A is shown in Figure – *Stress dependence on time*. At the initial time instant, point A corresponds to liquid phase of matter, and all the components of the stress tensor are negligible. Later on, when point A enters the phase change zone, radial and circumferential stresses start to increase linearly, and at a certain time instant ($t=1830$ s) crystallization of matter takes place at this point followed by a jump of all considered stresses. After completion of the phase change process, stress values come to the stationary level.

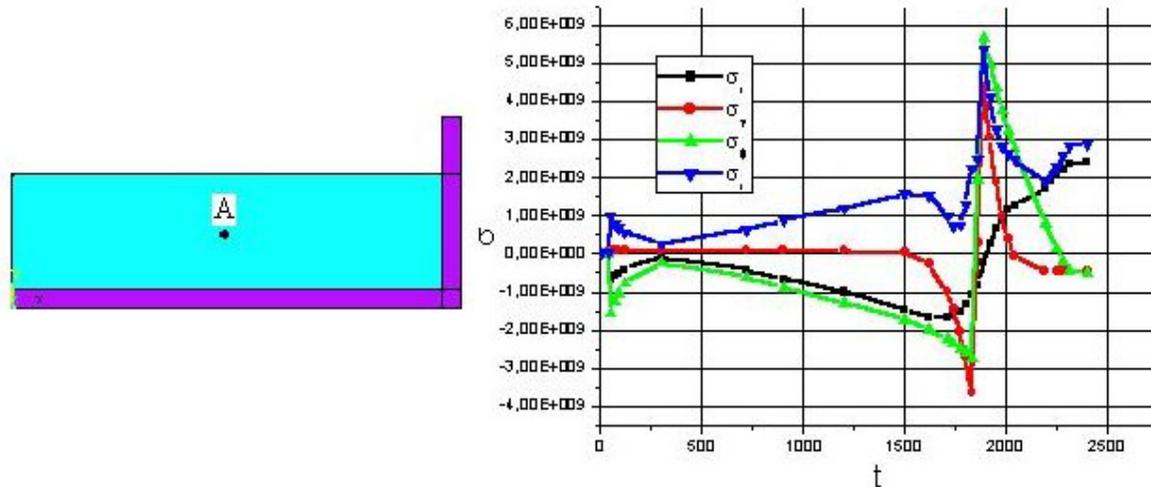


Figure 30 - Stress dependence on time

APDL Subroutine

The software, written in APDL-Lang and presented below is intended for transferring transient temperature field from the solved problem of thermal conductivity to the problem of thermoelastoplasticity.

```
*do,i,1,N
parresume
t=t+dttime
j=j+1
parsave,all
.....
ldread,temp,,,t,,thermal,rth
time,t
delttime,dttime,dmin(j),dmax(j)
nsubst,nsub,nmax(j),nmin(j)
lswrite,j
*enddo
```

Conclusion

The mathematical model of the liquid silicon oriented crystallization in the graphite mold was presented. During the simulation of the coupled (semi-coupled) thermoelasticity problem the transient temperature field, stresses and strain in a casting and a graphite mold at phase change and subsequent cooling was calculated.

This paper contains the results of researches implemented within a Bachelor Project.

Reference

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- 3) Cesari F. An enthalpy formulation of the conduction problem with phase changes, Computers&Structures, 1992.