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Thermal analysis of Germanium Crystal Growth using induction heating

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Abstract—.the objective of the present study is to develop a global simulation of an inductively heated crucible containing *Germanium* (***Ge***) **in a crystal growth** (*CZ*) **system, so as to predict the characteristics of the thermal field. The configuration should be optimized to get the appropriate thermalconditions.** A **special attention is given to the convective flows in the melt.** The **electro-magnetic, the thermal field, and fluid flow calculations are coupled to observe the shape of crystal-melt interface. Therefore, the effect of temperature gradients with various growth parameters, such as the current of** RF **coils, will be investigated.**

Keywords:
Crystal growth; Inductive heating; Numerical Model; Germanium

I. INTRODUCTION

Crystal growth is a complex process that involves heat transfer, convective flows in the melt phase, and stress in the growing crystal [1]. Induction heating is frequently used in order to supply the required heat to the crucible. This power is generated by induction, when a high frequency current is passed through the coils. Both fields penetrate the crucible to an extent that depends on the electrical conductivity of the material. The coil characteristics *(frequency, geometry)* can be optimized to reduce the energy consumption and ensure a controlled melting of the material. The axial symmetry of the geometry allows for a simplified 2D model representation in cylindrical coordinate system.

Different mechanisms of heat transfer coexist in the growth setup, including: conduction, radiation, and convection in the melt. Modeling of these is essential to understand and control the process [2-7]. Numerical tools are used: FEM software *COMSOL*, used to solve hydrodynamics and thermal equations, is coupled to Matlab which computes the Maxwell equations.

The thermal conditions in the system are studied by means of coupled induction heating and heat transfer. First the generated electromagnetic field is investigated. Then the temperature distribution in the whole system and the velocity of the melt will be calculated.

II. GERMANIUM CRYSTAL GROWTH

High purity germanium *(HP-Ge)* single crystals have many applications in semiconductor technology [8]. The material is initially melted in a crucible. Due to the axial temperature gradient, a seed crystal grows when it is pulled.At the beginning of the process, the temperature of the melt surface is adjusted so as it reaches the melting point (937°C). Then the seed crystal is slowly rotated and withdrawn to initiate the crystal growth. Seed rotation is used to improve the thermal symmetry and to drive forced convection in the melt [3].

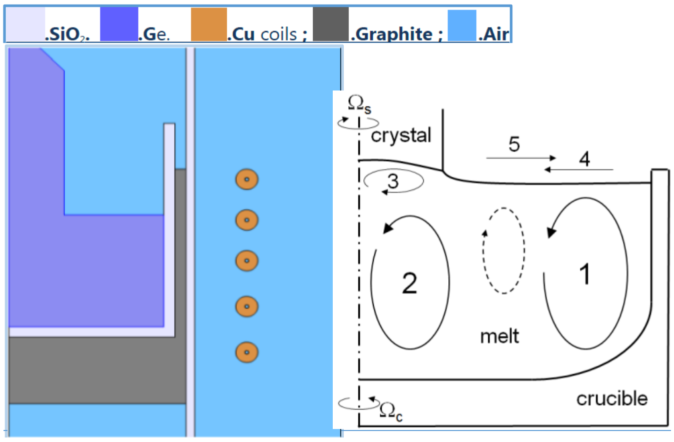


Fig. 1: Geometry *of* Model. (r) Melt convection due to: (1) Buoyancy, Forced convection –Coriolis (2), -Centrifugal (3), Marangoni (4), Gas flow (5)

Figure 2: Photo *of* crystal growth [7]

III- MODEL DESCRIPTION

Quasi-steady axisymmetric model

C*Z-is a well.known method in crystal growth, where* different mechanisms of heat transfer coexist (such as: convection/radiation). Modelling of these is essential to control the process. The physical phenomena involved in the simulation are induction heating, heat transfer, and fluid dynamics (convection flows that gives the radial and axial velocities in the melt).

Assumptions:

✓Steady state laminar flow;✓Incompressible Newtonian fluid;
✓No slip at the wall-liquid interface; ✓**Quasi-static approximation**

Navier Stoke's equation (Momentum Conservation)

$$\rho(\boldsymbol{u}.\nabla)\boldsymbol{u} \;=\; \nabla.\left[p\boldsymbol{I}+\mu(\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^T\right]-\rho b\boldsymbol{g}(T-T_0)+\overrightarrow{F_L} \qquad (1)$$

$\boldsymbol{u}$: Velocity of fluid, p: the pressure, μ : the viscosity, ρ: is the density
$\boldsymbol{g}$: Gravity. T: temperature (T_0: reference)
F_L: Lorentz force.

$$F_L=j\times B \qquad (2)$$

$\boldsymbol{J}$ is the current density. $\boldsymbol{B}$: *magnetic field*

Induction heating

The governing equations of electrodynamics are the *Maxwell* equations and Ohm's Law which can be combined to the induction equation.

Generalised Ohm's Law

$$\mathbf{J}=\sigma\left(-\nabla\phi+\mathbf{v}\times\mathbf{B}\right)$$

Conservation of charge

$$\nabla\cdot\mathbf{J}=0$$

σ : electric conductivity of the charge

Magnetic field equation:

$$j\mu_0\omega\,\sigma(T)\overrightarrow{A}+\nabla\times\left(\nabla\overrightarrow{A}\right)=\mu_0\sigma(T)\overrightarrow{grad}\,V \qquad (3)$$

Where:λ is the magnetic diffusivity. The induction equation describes the advection and diffusion of a magnetic field in a conductor.The resultant equations are based on the assumption that the magnetic field is time harmonic.

In *COMSOL's* notation [9] the volume force can be written as:
Fz = (d(mf.normB^2/mu0_const),z)/4.

Heat Transfer

–***Energy Conservation***:

Steady state is assumed during the crystal growth process. Under this assumption, the energy conservation may be written as

$$-\mathrm{div}\left(\mathrm{k(T)}\overrightarrow{grad}T\right)+\rho C_p\mathbf{u}.\overrightarrow{grad}T=\mathrm{Q_{th}}=\frac{1}{2}\sigma\omega^2\,\overrightarrow{\mathrm{A}}\,\overrightarrow{\mathrm{A}^*} \qquad (4)$$

Q_{th} : Heat losses.

A set of boundary condition must be formulated for the magnetic model. We imposed zero vector potential *(magnetic insulation)* on the limiting box. Normal induction field (=0) is imposed along the symmetry axis. Heat flux conservations are kept at all interior boundaries of adjacent domains.

Numerical modelling allows adjusting the temperature and the temperature difference along the crucible by the control of the current in the coil, by adjusting the position of the coil and by modifying the geometry.

Germanium	*Liquid*	*Solid*
Melting temperature, T_m (K)	**1209**	**1209**
Density, ρ (kg m^{-3})	**5553**	**5370**
Thermal conductivity, $\boldsymbol{k}$(W $m^{-1}K^{-1}$)	**39**	**17**
Specific heat capacity, C_p(J kg^{-1} K^{-1})	**393**	**380**
Latent heat of fusion, L_f (J. kg^{-1})	**46500**	**-**
Viscosity, μ (Pa. s)	**$27\ 10^{-4}$**	**-**
Thermal expansion, b (K^{-1})	**$2\ 10^{-5}$**	**$2\ 10^{-5}$**

	Density	C_p	K (W m^{-1} K^{-1})
Graphite	**1860**	**918**	**25**
Quartz	**1930**	**1060**	**4**
Cu	**8700**	**385**	**400**
Argon	**1.623**	**521**	**0.016**

Arg. viscosity, (Pa. s): $2.125\ 10^{-5}$

TABLE I: Physical properties used in the simulation

III. RESULTS

Heat transfer characteristics are determined, and the results graphically depicted. The computed thermal field is highlighted, zooming inside the hot zone (**Fig. 3**). We can observe that, even if the current is very intense in the coil, the temperature is close to ambient thanks to the water cooling system. On the contrary, the temperature in the charge is high and close to the melting point of the material due to eddy currents and the Joule effect. The other parts are heated by radiation.

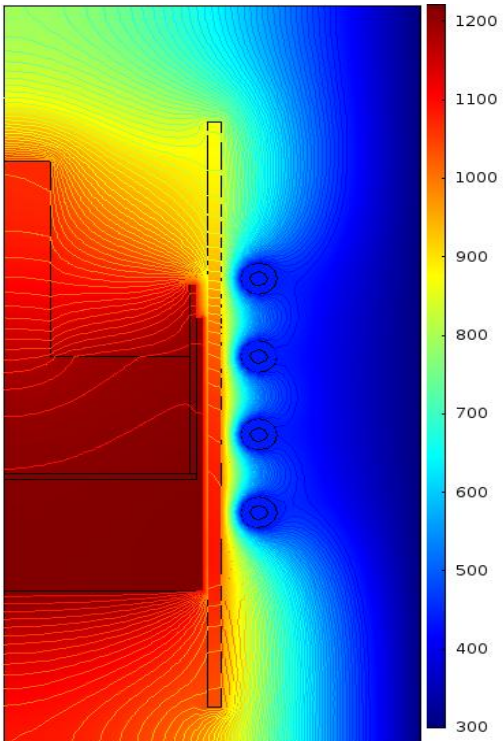
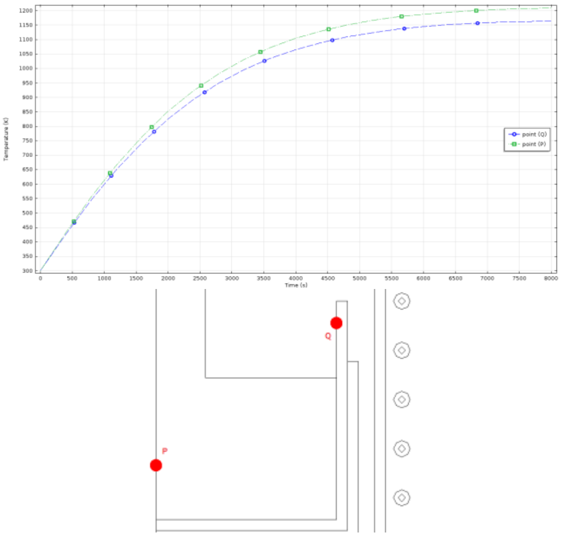


Figure 3: Temperature distribution [K]



The resulting current density is plotted in the following figure, together with the magnetic field flux lines (**Fig. 4**). We can see that the maximum current density is located in the coil domains. Inside the crucible, the magnetic field flux lines are highly deformed and an eddy current flowing in the opposite direction is induced. The in-phase magnetic flux in liquid dissipates mainly close to the crucible wall. These contribute to the Lorentz force which is one of the main contributions to the convection patterns in the melt phase.

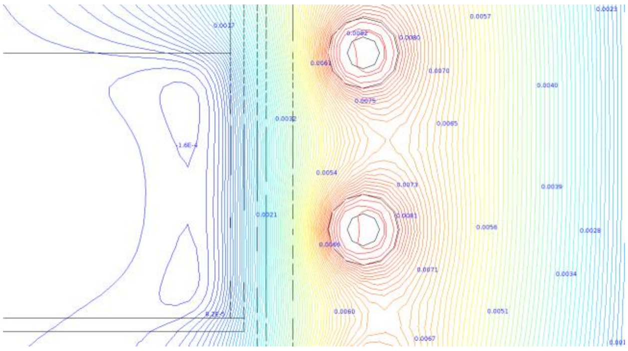


Figure 4: *Magnetic vector potential contours, phi component* $A_i\,[Web/m]$

Melt convection

Determining the melt flow pattern is essential to find a relation to the crystal growth behavior. Therefore, it is necessary to understand its origin and the dependency of the different forces acting on the molten zone. Several convective phenomena, such as buoyancy and forced convection can occur depending on the process conditions [**1**].

1. Buoyancy

First, it is necessary to know how the fluid moves only due to the natural convection, driven by the heat transferred from the walls of the crucible to the melt. To calculate that, the rotation and the pulling rates of the crystal are set to zero. As expected, the flow moves upward along the crucible walls. This is because the melt expands and becomes less dense when heated by the walls of the crucible. It cools down and becomes denser while flowing along the surface. As can be seen, there are two vortices in the melt (**Fig. 5**).

Both of them are induced by the thermal buoyancy force. The upper vortex circulates inward along the melt free surface, while the lower one flows in the opposite direction.

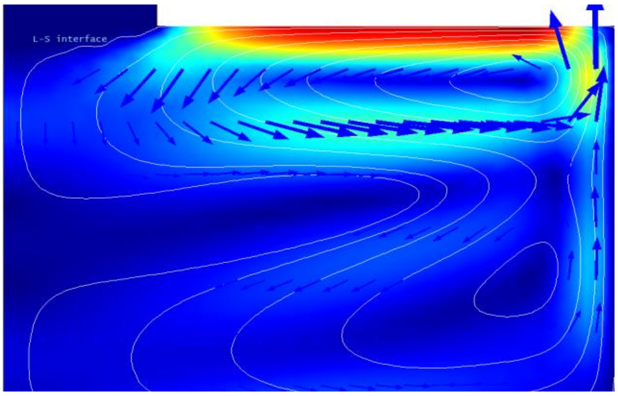


Figure 5: velocity mapping and streamlines in the Ge melt

The velocity of fluid is significantly higher at the surface than in the volume. The fluid on the free surface *(hotter)* is moved to the low-temperature regions by the gradient of surface.

2. Magneto hydrodynamic flow

The rotational part of the Lorentz force accelerates the fluid in the direction of the magnetic field gradient. This Lorentz force creates a double vortex structure in the melt causing the melt at the free surface to flow from the crystal to the crucible wall, i.e. against the basic buoyant flow direction (**Fig. 6**).

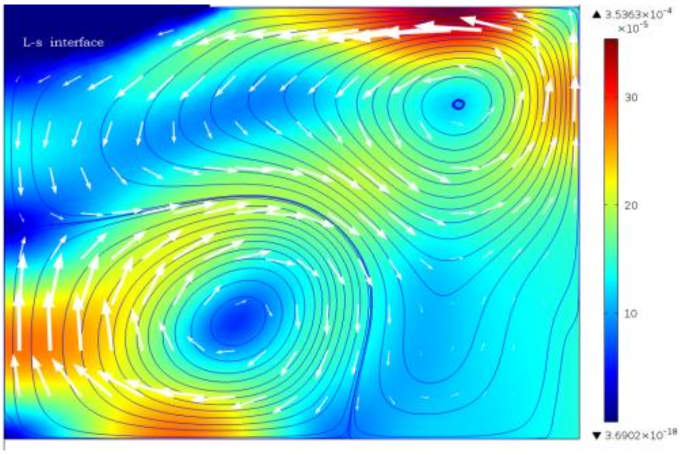


Figure 6: velocity field in the Ge melt, taking into account the Lorentz force

Conclusion

We have performed a global simulation of heat transfer to study the crystal growth of *Germanium* in a CZ configuration. Thermal and velocity fields were calculated. The effect of temperature distribution on the melt convection patterns was pointed out. The variations of interface type were attributed to variations in temperature gradients and to convection currents in the liquid phase. The coil characteristics (frequency, current, geometry) as well as the geometry can now be optimized to reduce the energy consumption and ensure a controlled melting of the material.

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REFERENCES

[1] P. RUDOLPH, Transport phenomena of crystal growth – Heat and mass transfer. AIP Conference Proceedings, vol. 1270 (2010) 107

[2] M. TAVAKOLI, A. SADEGHI, Global simulation of a CZ furnace during different stages of germanium crystal growth, Crystal Eng. Com 18 (2016) 3942

[3] F. Mercier, Coupled heat transfer and fluid dynamics modeling of SiC solution growth, J. Crystal Growth 312 (2010) 155

[4] R. Faiez, Radiative Heat Transfer and Thermo-capillary Effects on the Structure of the Flow during Czochralski Growth of Oxide Crystals, Advances in Chemical Engineering and Science,5 (2015) 389-407

[5] Young Yoon, M.-Hyun Lee, "Process design for SiC single crystal based on multiphysics modeling", J. of the Korean Crystal Growth and Technology 26 (2016) 8-13

[6] M. Tavakoli, Numerical modeling of induction heating in crystal pulling method; J. Modern Physics 1 (2014) 41

[7] Czochralski Crystal growth control by the crucible weighing method"I. HAMADAS, A. MANSERI, D. OUADJAOUT, A. HAKEM, J. CHAMINADE, IEEE Conference Publications (2016) 7th International Renewable Energy Congress (IREC) 1- 4

[8] Performance Differences of mono- vs. Polycrystalline Germanium for Optical Applications *D. Hibbard. SPIE photonics (2013)*

[9] *COMSOL as a tool for studying Magneto-Hydro-Dynamic effects in liquid metal flow under transverse magnetic field. S. SAHU* (2013) COMSOL conference.