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Computational analysis of heat transfer, thermal stress and dislocation density during resistively Czochralski growth of germanium single crystal

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ABSTRACT

In this paper, a set of numerical simulations of fluid flow, temperature gradient, thermal stress and dislocation density for a Czochralski setup used to grow IR optical-grade Ge single crystal have been done for different stages of the growth process. A two-dimensional steady state finite element method has been applied for all calculations. The obtained numerical results reveal that the thermal field, thermal stress and dislocation structure are mainly dependent on the crystal height, heat radiation and gas flow in the growth system.

1. Introduction

Today, bulk germanium is a key material for an extensive range of industrial applications including infrared (IR) lenses and windows (thermal imaging), nuclear detectors, opto-electronic and fibre-optic systems and solar cell components. Since germanium has some attractive properties for example, charge carriers with higher mobility compared to silicon (electrons and holes: two and four times, respectively), high absorption coefficient in the wavelength range 8000–15500 Å, low absorption and high transmission of infrared radiation in 2–15 μm range and high refracting index (∼4). It can also help for solving of some special problems in the development of nano-scale transistor structures [1]. The total worldwide consumption of germanium is estimated to be about 100 ton/year.

The most common method of growing IR-grade single germanium crystal is the Czochralski (CZ) process. Using this method, the crystal grows slowly under pulling from the molten material. The melt and gas motion is an important parameter for crystal growers because it determines the transport of mass, heat and impurities to/from the grown crystal. The crystal quality or defect formation and dislocation propagation in grown crystal is directly connected to the thermal history of the growth process, the crystal and crucible rotation, the pulling rate and the cooling procedure [1–8].

Usual prerequisites for IR optical-grade Ge crystals is absorption coefficient < 0.02 cm^{-1} at room temperature, very low non-homogeneity of the refractive index $\Delta n < 10^{-4}$ (i.e., optical uniformity and isotropy) and minimized inherent birefringence (<1 μm cm^{-1}). Furthermore, to achieve these conditions, the residual stresses in the grown crystal must be diminished [1]. To decrease the thermal stresses, the crystallization front must be retained as flat as possible during the CZ growth process, related to an almost reducing radial temperature gradient within the crystal. These conditions can be carried out by exact setup design; precise and stable growth conditions and apply of suitable heat shields and/or after-heaters above the melt surface.

Nowadays, mathematical modeling of crystal growth processes has reached a point where it can be successfully applied to study the fundamental phenomena (physical, chemical and mechanical) of the process. This method is an effective tool to make desired variations in the existing processes and setups, and to develop and design novel systems for growth new crystals [7–16].

Despite the wide spread use of Ge, unfortunately, there have been little reports of computer modeling for CZ growth of germanium. Crowley [17] described a mathematical approach of the heat transfer for the Ge Czochralski method including moving

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boundaries and the melt surface meniscus using the enthalpy method. Dupret et al. [18] performed a quantitative prediction of the temperature gradient and the crystallization front during growth of germanium crystal using radiative exchanges with the presumption of diffuse surfaces. Bogaert and Dupret [11,19] simulated the time-dependent Cz growth of Ge crystal taken into account heat transport via conduction and diffuse grey radiation, in and between all the exposed surfaces without the melt convection. Bykova [20] calculated a 2D transient problem of germanium crystal growth by the AHP method under microgravity conditions and showed that axial microaccelerations will have no influence on the weakly forced melt flow along the melt–crystal interface. Abbasoglu [21] carried out a time-dependent three-dimensional numerical simulation to investigate the influence of crystal and crucible rotations on the fluid flow and the radial segregation of Si during the growth of Ge_x Si_{1-x} crystals by the Cz technique under microgravity conditions. Recently, Honarmandnia et al. [22,23] have performed a 2D global simulation of an RF Czochralski system for different stages of Ge crystal growth in order to predict and analysis of thermal field, the crystallization interface and thermal stresses of the grown crystal.

The present study involves the application of a global numerical analysis to a CZ growth furnace of IR optical-grade Ge single crystal with resistive heating system for different stages of the growth process. The goal is to predict accurately, (1) the thermal–hydrodynamic behavior of the melt and gas, (2) the shape of the crystal–melt interface, and (3) the thermal and thermoelastic stress behavior of the grown crystal. Furthermore, a first-order approximate of the dislocation density in the grown crystal is presented. The present study can be a useful source of information for the crystal growers in the fields of thermal gradient, heat transport and thermal stress structure during and shortly after the growth process. This detailed information is crucial for the reduction of thermal stresses at the time and immediately after the growth process, which is necessary for obtaining high optical uniformity and minimized birefringence of the IR germanium crystals. The obtained results are specifically important in processes of semiconductor crystal growth industry especially Czochralski germanium crystal growth which currently focuses on the high pure, IR optical-grade and dislocation free ingots with outstanding dopant control.

2. Modeling approach

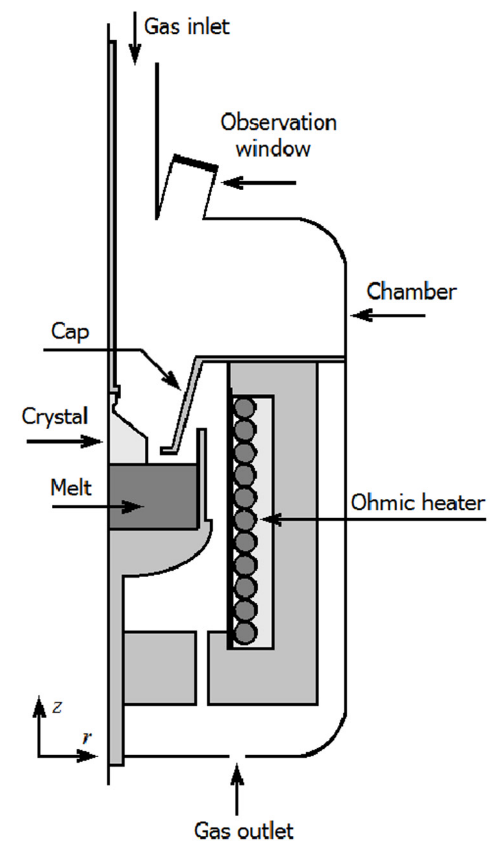
2.1. Governing equations and boundary conditions

2.1.1. Thermal field

The considered CZ growth setup (which is used to growth germanium) consists of a graphite crucible, a graphite cap, thermal insulation, resistance-coil and chamber, Fig. 1. Our mathematical model includes the following basic assumptions which arise from observation and measurement in our lab: (1) The growth setup is in steady state and axially symmetric, (2) Fluid parts (i.e., melt and argon gas) are incompressible Newtonian fluids agreeable the Boussinesq approximation, (3) The flow of the melt and gas is laminar, (4) Viscous dissipation is negligible, (5) The radiation heat transfer is governed only by surface to surface radiation. The assumption of laminar melt and gas flow arises from two reasons, (1) Our observation and measurement in the lab, and (2) Calculation of the Rayleigh number (Ra) of the melt and gas which is less than 10^9 (critical value for transition to turbulence flow [24]).

The governing equations for the fluid parts (melt and gas) are the conservation equations for mass, momentum and energy, which have the following forms [13,14];

(a)



(b)

Fig. 1. (a) A photo of the insight of Czochralski setup during the growth process, and (b) Sketch of the furnace used for Ge growth.

(a) Continuity equation:

$$\nabla.\vec{V} = 0 \qquad (1)$$

(b) Fluid flow:

$$\rho\vec{V}.\nabla\vec{V} = -\nabla p + \mu\nabla^2\vec{V} + \rho\beta g(T - T_0)\hat{e}_z \qquad (2)$$

(c) Heat transport via conduction and convection:

$$\alpha\nabla^2 T - \vec{V}.\nabla T = 0 \qquad (3)$$