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Grown-in Defects of InSb Crystals: Models and Computation

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Abstract. In this paper, we present a model for grown-in point defects inside indium antimonide crystals grown by the Czochralski (CZ) technique. Our model is similar to the ones used for silicon crystal, which includes the Fickian diffusion and a recombination mechanism. This type of models is used for the first time to analyze grown-in point defects in indium antimonide crystals. The temperature solution and the advance of the melt-crystal interface, which determines the time-dependent domain of the model, are based on a recently derived perturbation model. We propose a finite difference method which takes into account the moving interface. We study the effect of thermal flux on the point defect patterns during and at the end of the growth process. Our results show that the concentration of excessive point defects is positively correlated to the heat flux in the system.

Key words: Crystal growth; Czochralski technique; point defects; recombination; thermal flux; finite difference method.

1 Introduction

Indium antimonide (InSb), a compound semiconductor which is useful as an infrared detector and filter, has attracted considerable attention over the last several years. Due to thermal fluctuation and/or presence of impurities during the crystal growth process, the structure of the crystal posses various imperfections, known as defects. Among various types of defect, the basic ones are the point defects (interstitial, vacancy, interstitialcy).

Most of the previous work on point defects has been done for silicon crystals. Taking convective flux, diffusive flux and recombination of interstitials and vacancies into account, Voronkov [21,22] proposed a model of micro-defect formation in silicon and authors in [8,

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13–15] followed the similar models. While many researchers [4,5,11,12,18] have improved the model by adding the reduced heat transfer effects, Sinno et al. [17] have further added the effect of nucleation of excess vacancies or excess interstitials. While the general principle is similar for different types of crystals, material properties may have an impact on the formation and dynamics of point defects.

In this paper we extend the Voronkov model [22] to indium antimonide crystal grown by the CZ technique. The main objective of the paper is to compute the distribution of point defects and their supersaturation values by solving the model equations numerically. We will exam the effect of controlling parameters such as the heat fluxes at the gas/crystal and melt/crystal interfaces on the point defects distribution. The rest of the paper proceeds as follows. We present our basic model for two types of point defects in Section 2. A numerical method for solving the model equations is proposed in Section 3. Numerical results for the basic model are given in Section 4 and we finish the paper by a short discussion in Section 5. A generalization of the basic model is given in the Appendix.

2 Basic model

To simplify the computation, we neglect the impurity atoms and interstitialcy defects. Furthermore, we consider only neutral species of point defects and neglect charged species and focus on the distribution of two types of point defects, namely interstitial and vacancy. Taking convective flux, diffusive flux as a Fickian diffusion and recombination reaction between interstitial and vacancy into account, mathematical model governing the point defects is of the reaction-diffusion type, written as

$$\frac{\partial C_I}{\partial t} = \nabla \cdot (D_I \nabla C_I - \vec{f}_p C_I) - R_{IV}(C_I C_V - C_I^e C_V^e), \tag{2.1}$$

$$\frac{\partial C_V}{\partial t} = \nabla \cdot (D_V \nabla C_V - \vec{f}_p C_V) - R_{IV}(C_I C_V - C_I^e C_V^e), \tag{2.2}$$

where C_I and C_V are volume concentrations of interstitial and vacancy point defects, respectively. R_{IV} is the temperature dependent reaction rate, which determines how fast the recombination is taking place. It can be expressed as a function of the mobility of point defects and a free energy activation barrier as

$$R_{IV} = 4\pi a_r (D_I(T) + D_V(T)) e^{-\frac{\Delta G_{IV}}{k_B T}},$$

where a_r is an effective capture radius, k_B, the Boltzmann's constant and ΔG_{IV}, the free energy barrier against recombination of interstitial and vacancy. C_j^e, $j = I, V$ are the equilibria of C_j for a given temperature T, given by the formula

$$C_j^e = C_j^0 e^{-\frac{E_{jf}}{k_B}\left(\frac{1}{T} - \frac{1}{T_0}\right)}$$