DISTRIBUTION OF BORON-IMPURITY IN Ge-Si BULK SINGLE CRYSTALS GROWN FROM THE MELT

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ABSTRACT

A problem of B-impurity distribution in GeSi crystals grown by conventional Czochralski method has been solved theoretically in consideration of the linearly dependence of the impurity segregation coefficient on the melt composition. A considerable influence of the B-impurity segregation coefficient changing during the growth process on the axial impurity concentration profile in Ge-Si crystals is shown. The obtained equations determine the operational parameters and optimum processing conditions in preparing bulk single crystals of Ge-Si with a desired impurity concentration profile.

Keywords: Ge-Si, Czochralski method, Impurity, Segregation

I. INTRODUCTION

Impurity-doped Si and Ge single crystals are the basic materials of the modern microelectronics industry. The interest to investigate GeSi –solid solutions goes bask to the fifties due to same outstanding material properties. Bulk single crystals of GeSi solid solutions with a uniform and/or compositionally graded profiles were grown recently by the Czochralski, Bridgman, zone-melting, multicomponent zone-melting methods [1-15]. The further investigations have been developed to study a problem of the shallow impurities distribution in bulk GeSi crystals, grown from the melt [8,10,14]. Among the chemical elements, used as a shallow impurity in these semiconductors, the elements of the III and V groups of the periodical system take an important place. Small ionization energy and high solubility of these impurities in the matrix define the electric properties of the semiconductors in a wide temperature range.

In this paper, a problem of Boron- impurity distribution in GeSi crystals grown by conventional Czochralski method has been solved theoretically in consideration of the dependence of the impurity segregation coefficient on the melt composition. The purpose is to estadlish the operational parameters and optimum processing conditions in preparing B-doped GeSi crystals with a desired impurity distribution profile along the crystallization axis.

II. RESULTS AND DISCUSSION

As an example, the curve1 in Fig.1 shows the calculated Si composition profiles in a GeSi bulk crystal grown by Czochralski method from the melt with starting composition 50 at.% Si.

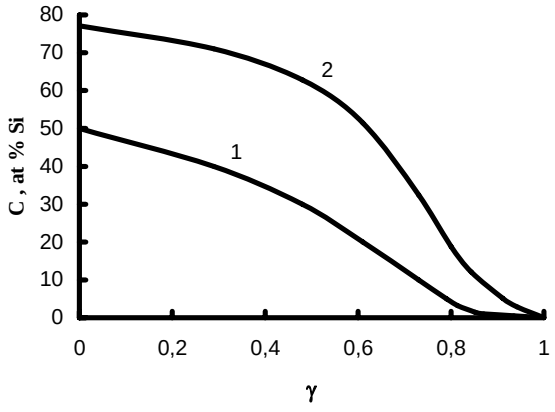

Fig.1. Si composition in the crystal (curve 1) and in the melt (curve 2) as a function of γ . A starting composition of the Ge-Si melt is 50 at.%Si

The curve was calculated numerically using the data of [6] and the equilibrium segregation coefficients of Si estimated from the continuous calculation of the Ge-Si phase diagram [2]. The Si content is maximal at the seed end and decreases approaching zero at the tail of the ingot. The curve 2 demonstrates the corresponding Si

concentration in the melt during the growth process. In all cases the crystals grown by the conventional Czochralski method have compositionally graded composition along the crystallization axis.

The problem of B-impurity distribution in GeSi crystals with graded composition shown in Fig.1 was solved under the following standard assumptions. At the growth front, the crystal and the melt are in equilibrium; the crystallization front is planar; the diffusion of the components and boron impurity and the convection in the melt provide homogeneity of the liquid phase throughout in the entire volume; the diffusion of B atoms in the solid phase is negligible; B-impurity distribution coefficient changes linearly with the composition of the Ge-Si melt, due to the virtual model consideration.

Below, the following designation are used: V_0 and V_l are the initial and current GeSi<B> melt volumes; V_c is the volume of the melt solidifying per unit time; C_l^0 and C_l are the Boron concentrations in the liquid and solid phases, respectively; C is the total amount of B-impurity in the melt; C_B is the concentration of B-impurity in the crystal; K_B^{GeSi} is the equilibrium segregation coefficient of Boron in the current moment, t is time.

With these designations, we have

$$C_l = \frac{C}{V_l} \quad and \quad \frac{dC_l}{dt} = \frac{\dot{C}V_l - \dot{V}_l C}{V_l^2} \qquad (1)$$

Given that V_c is independent of time and $C_B = C_l K_B^{GeSi}$, we have

$$V_l = V_0 - V_c t, \;\; \dot{V}_l = -V_c, \;\; \dot{C} = -V_c C_l K_B^{GeSi} \qquad (2)$$

Substituting Eq.(2) into (1), and integrating we obtain

$$\int_{C_l^0}^{C_l} \frac{dC_l}{C_l - C_l K_B^{GeSi}} = \ln \frac{V_0}{V_0 - V_c t} \qquad (3)$$

Assuming that the solid and liquid densities are equal, we can rewrite Eq. (3) in terms of the fraction of the solidified melt, $\gamma = V_c t / V_0$:

$$\gamma = 1 - \exp\left[- \int_{C_l}^{C_l^0} \frac{dC_l}{C_l (K_B^{GeSi} - 1)} \right] \qquad (4)$$

As has been mentioned above, B-impurity distribution coefficient changes linearly with the composition of the Ge-Si melt, and we have:

$$K_B^{GeSi} = K_B^{Ge} - C_{Si}^l (K_B^{Ge} - K_B^{Si}) \qquad (5)$$

where C_{Si}^l is the silicon fraction of the melt; K_B^{Ge}=17 and K_B^{Si}=0,8 [10] are the equilibrium Boron segregation coefficients in Ge and Si respectively.

Fig.2 shows K_B^{GeSi} as a function of the fraction of the solidified melt (γ) obtained from the C_{Si}^l vs γ data (Fig.1) and equation (5).

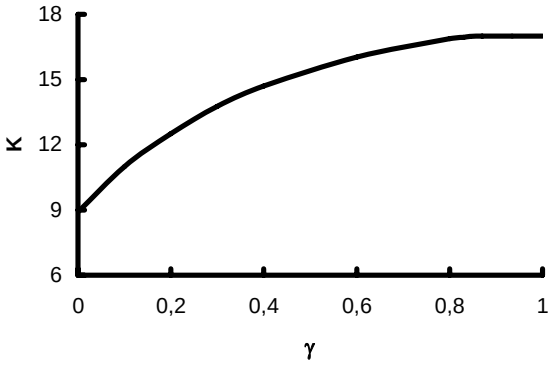

Fig.2. Boron segregation coefficient in Ge-Si system as a function of γ calculated from the data of Fig.1 and equation (5).

The curve furnished by Fig. 2 demonstrates that K_B^{GeSi} depends on γ in complicated manner and can not be approximated by a simple function. But the data of the Fig.2 allow to evaluate the integral in equation (4) using the Boron equilibrium segregation coefficients with corresponding values of γ. In this way C_l or $C_B = K_B^{GeSi} C_l$ can be determined as a function of γ and Boron profile in the crystal can be plotted against the fraction of the solidified melt. As an example, the curve (2) in Fig.3 shows the calculated B concentration profile in Ge-Si crystal grown from Ge-Si melt with starting composition 50 at.% Si and Boron concentration of $1x10^{16} sm^{-3}$).

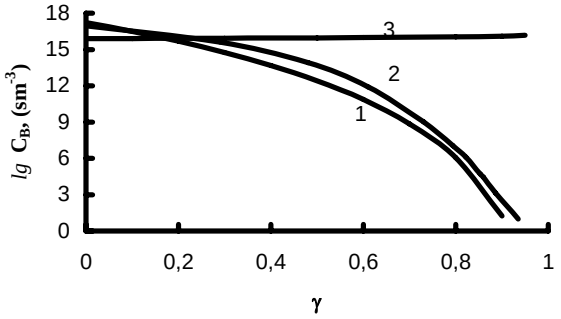

Fig.3. Boron concentration profile in Ge (curve 1) and Si (curve 3) crystals and in Ge-Si (curve 2) crystal grown from the melt with a starting composition Ge(0.5)Si(0.5). Boron starting composition in the melt is $1x10^{16} sm^{-3}$ in all cases.

The B content is maximal at the seed end and decreases approaching zero at the tail end of the crystal. The slope of the curve is smaller in the seed portion than in the tail part of the ingot. This difference arises from the large

increase in K_B^{GeSi} with decreasing Si contend in the melt (Fig.1).

For comparison, the curves (1) and (3) in Fig.3 show the Boron concentration profile in Ge and Si crystals grown from the melt with the same starting B content as in the case of the Ge-Si melt. These curves were calculated using Pfann formula [10] in consideration of a complete mixing regime. One can seen than behavior of B concentration profile in Si differ from that one in Ge and Ge-Si crystals and increases along the crystallization axis. The reason $K_B^{Si}<1$, when K_B^{Ge} and $K_B^{Ge(0.5)-Si(0.5)}>1$.

For some applications a uniform impurity distribution in crystals is needed. For growth such a crystal an already B-doped Si feeding ingot can be used [1].

III. CONCLUSION

The above mentioned main results can be summarized as follows:

A problem of B-impurity distribution in GeSi crystals grown by conventional Czochralski method has been solved theoretically in consideration of the linearly dependence of the impurity segregation coefficient on the melt composition.

A considerable influence of the B-impurity segregation coefficient changing during the growth process on the axial impurity concentration profile in Ge-Si crystals is shown.

The obtained equations determine the operational parameters and optimum processing conditions in preparing bulk single crystals of Ge-Si with a desired impurity concentration profile.

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