DISTRIBUTION OF COMPONENTS IN Si-Ge CRYSTALS GROWN BY ZONE LEVELLING METHOD

G.Kh. AZHDAROV

Institute of Physics of Academy of Sciences of Azerbaijan, Baku, G.Javid 33, 370143

A. VARILCHI, T. KUCHUKOMEROGLU, M. ALTUNBASH, A.I. KOBYA

Department of Physics, Faculty of Arts and Sciences, Karadeniz Technical University, 61080-Trabzon, Turkey

A component distribution in Si-Ge bulk crystals grown by zone levelling technique has been analyzed theoretically with a view to estimating operational parameters in preparing mixed crystals with a desired uniform and/or graded composition profiles. A numerical model, using the equilibrium distribution coefficient defined in the phase diagram, capable of predicting the components redistribution in Si-Ge crystal at any stage of zone leveling growing is proposed. Compositional profiles of Si-Ge crystals for a number values of operational parameters, such as molten zone length and a starting ingot composition, are calculated and discussed. It was found that Si concentration profile in Si-Ge crystal as a function of zone length changes considerably from fully graded to almost uniform along the growth direction. Obtained results allow operational parameters in preparing Si-Ge mixed crystal to be estimated.

1. Introduction

During the last few years bulk single crystals of Si-Ge system have been grown using different methods, including the zone levelling technique [1-4]. The component distributions in Si-Ge crystals grown by the Czochralski method were calculated recently, using a numerical model [5]. A good agreement with the experimental data was obtained. The results reported by the authors of [5] show that a compositional profile in Si-Ge crystals is close to that a completely mixed melt.

In the present paper a numerical model has been developed for the evaluation of the longitudinal components distribution in Si-Ge alloys grown by the zone levelling method. The calculations are based on the data obtained from the phase diagram and on a model of a completely mixed melt. The purpose is the establishing of operational parameters in preparing Si-Ge crystals with a desired uniform and/or compositionally graded profiles.

2. Theoretical Background

A quantitative evaluation of the component distribution in Si-Ge alloys was carried out under the following standard assumptions [6]. At the growth front, the crystal and the melt are in equilibrium. The growth front is always planar. Diffusion in the melt is fast enough that the melt composition is uniform. Interdiffusion in the solid phase is negligible. An average composition of the initial Si-Ge polycrystalline ingot is macroscopically uniform throughout.

Below the following designations are used: V_m^0 and V_m are the initial and current melt volumes in molten zone; V_c and V_i the volumes of the melt solidifying and the ingot solving per unit time; C_c, C_i and C_m are the Si concentrations (atomic fractions) in the crystal, initial ingot, and molten zone, respectively; C_m^0 is the Si content in the molten zone at the start of growth; C is the total amount of Si in molten zone; K is the equilibrium distribution coefficient defined in the phase diagram; t is time; L and l are the lengths of the ingot and molten zone, respectively.

With the mentioned designations, we have

$$C_m = \frac{C}{V_m}, \qquad \frac{dC_m}{dt} = \frac{\dot{C}V_m - \dot{V}_m C}{V_m^2} \tag{1}$$

and

$$V_m = V_m^0 - (V_c - V_i)t \tag{2}$$

Given that V_c, V_i and l are independent of time for the ingot portion along the length up to the beginning of the tail molten zone, we have

$$V_m = V_m^0, \quad C_m^0 = C_i$$

and

$$\dot{C} = -V_c C_c + V_i C_i = V_c C_m K + V_i C_m^0 \tag{3}$$

Substituting (3) into (1), separating the variables, and integrating, we obtain:

$$\int_{C_m^0}^{C_m} \frac{dC_m}{C_m^0 - C_m K} = \frac{V_c t}{V_0} = \frac{z}{l} \tag{4}$$

Here z is the length of a growing crystal at the moment t. To take the integral in (4), one should know K as a function of C_m. fig.1 shows the equilibrium distribution coefficient K of Si-Ge alloy as a function of the composition defined in the phase diagram [7]. As follows from fig.1 K depends on melt composition in complicated manner and can not be approximated by a simple function. The integral in (4) can be evaluated numerically using K estimated from the continuous calculation of the phase diagram (fig.1).

For the tail portion of the ingot

$$V_m = V_m^0 - V_c t, \qquad \dot{V}_m = -V_c,$$

and
$$\dot{C} = -V_c C_m K \tag{5}$$

Substituting (5) into (1) and integrating, we obtain:

$$\int_{C_m^0}^{C_m} \frac{dC_m}{C_m^0 - C_m K} = \ln \frac{V_m^0}{V_m^0 - V_c t} \tag{6}$$

Where C_m^0 is the initial composition of Si in the tail molten zone, The equation (6) can be rewritten in term of the solidified melt in the molten zone; $\gamma = V_c t / V_m^0$

$$\gamma = 1 - \exp\left(- \int_{C_m}^{C_m^0} \frac{dC_m}{C_m K - C_m} \right) \tag{7}$$

As in the case of the equation (4) the integral in (7) can be evaluated numerically and Si profile in the tail portion of the crystal can be plotted against γ.

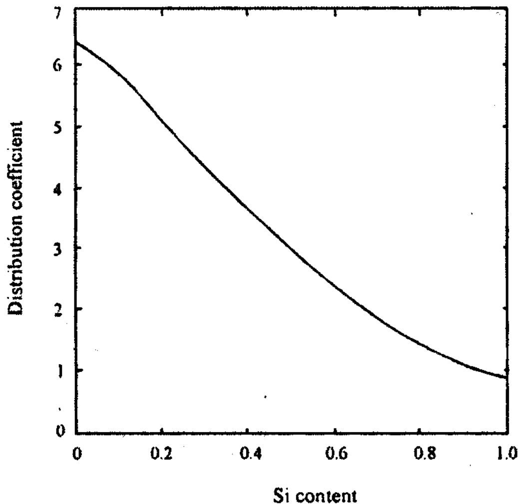

Fig.1. Equilibrium distribution coefficient K defined in the phase diagram [7].

3. Results and Discussion

Composition profile of Si-Ge crystals calculated for four C_i values using the equations (4) and (7) are shown in Fig.2. Here $l=L/10$ is considered. In all cases, the Si content is maximal at the beginning and then decreases approaching a uniform composition $C_c=C_i$. A uniform composition changes into a graded at the tail portion of a crystal. The length of this part for all considered compositions is l. Here the Si concentration decreases during growth approaching zero at the tail end of the ingot. The length of the compositionally graded top part of crystals depends on C_i because the segregation coefficient changes with the melt composition. A compositional gradient in the tail part of crystals decreases as C_i decreases because the length of molten zone is fixed.

As follows from the curves in fig.2, a Si concentration profile in a crystal can be controlled by varying the molten zone length. As an example, fig.3 illustrates the calculated Si concentration profiles in Si-Ge crystals for five l values. A starting composition of all ingots is $Si_{0.20}Ge_{0.80}$. For the case of $l=L$ (curve 1) a compositional profile of the crystal was calculated using equation (7) only. In fig.3, the results furnished by the curves demonstrate the efficiency of the operational parameter l on the components redistribution during zone levelling growth of Si-Ge. We can see that the length of compositionally graded and uniform portions of the crystals in a wide range are defined by the value of molten zone length.

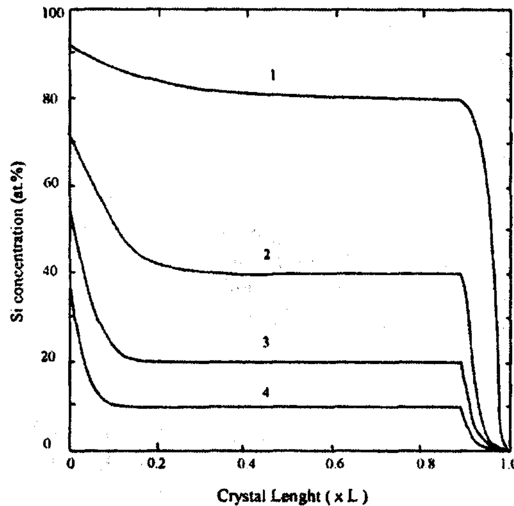

Fig.2. Longitudinal Si concentration in Si-Ge crystals grown by zone levelling method. Molten zone length is $l=L/10$. Starting composition of ingots are (1) C_i=80, (2) 40, (3) 20, and (4) 10 at. %Si.

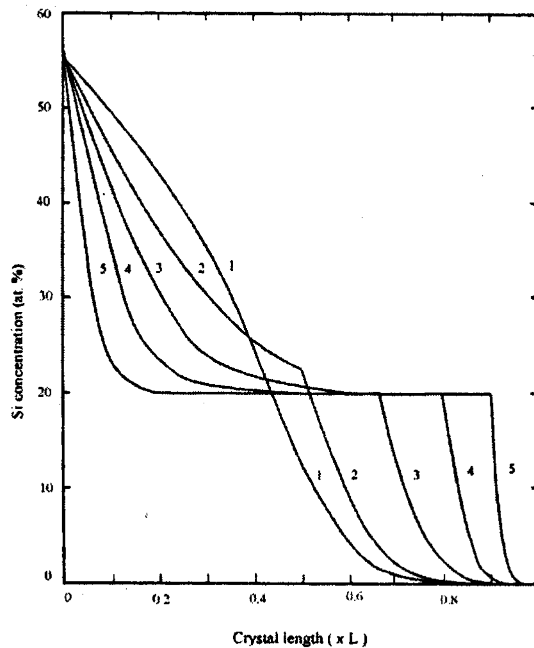

Fig.3. Longitudinal Si concentration in Si-Ge crystals grown by zone levelling method from a starting ingot $Si_{0.20}Ge_{0.80}$. Molten zone lengths are (1) $l=L$, (2) $L/2$, (3) $L/3$, (4) $L/5$ and (5) $L/10$.

A family of curves in fig.2 and fig.3 shows that a numerical model can establish operational parameters and optimum

processing conditions in preparing Si-Ge alloys with a desired uniform and/or graded compositions.

4. Conclusion

The composition in Si-Ge alloy grown by the zone levelling technique has been analyzed theoretically. A numerical model capable of predicting the components redistribution in a crystal at any stage of a zone levelling growing is proposed. It was found that a composition profile in Si-Ge alloy as a function of molten zone length changes in a wide range from fully graded to almost uniform along the growth direction. Obtained results show that the numerical model can estimate operational parameters, such as a molten zone length and a starting ingot composition, in preparing Si-Ge crystals with desired uniform and/or compositionally graded profiles.

Acknowledgements

This work was supported by NATO-CP Advanced Fellowships and The Scientific and Technical Research Council of Turkey.

[1] *A.Barz, P.Dold, U.Kerat, S.Recha, K.W.Benz, M.Franz, K.Presse.* J.Vac. Sci. Technol. B, Microelectron Nanometer Struct. 16,1998, 1627.
[2] *D.Biss, B.Demczyk, A.Anselmo, J.Bailey.* J. Crystal Growth 174 ,1997, 187.
[3] *J.Wollweber, D.Schulz, W.Schroeder.* J. Crystal Growth 158, 1996, 166.
[4] *J.Wollweber, D.Schulz, W.Schroeder.* J. Crystal Growth 163, 1996, 243.
[5] *P.G.Azhdarov, N.A.Agaev.* J. Inorganic Materials 35, 1999, 763.
[6] *V.M. Glazovand, V.S. Zemskov.* Fiziko-khimicheskie osnovy legirovaniya poluprovodnikov (Physicochemical Principles of Semiconductor Doping), Moscow: Nauka, 1967.
[7] *R.W.Olesenski, J.C.Abbaschian.* Bull. Alloy Phase Diagram 5, 1984, 180.

H.X. Əjdərov, Ə. Varilçi, T. Kiçikömeroğlu, M. Altunbaş, A.I. Kobya

ƏRİNTİ ZOLAQ ÜSULU İLƏ ALINAN Si-Ge KRİSTALLARINDA KOMPONENTLƏRİN PAYLANMASI

Bircinsli və ya dəyişən tərkibli Si-Ge kristallarının alınma texnologiyasının optimal parametrlərinin müəyyən edilməsi məqsədi ilə işdə ərinti zolaq üsulu ilə alınan bu kristallarda komponentlərin paylanma məsələsi analiz edilib. Ərinmiş zolağın uzunluğu və materialın ilkin tərkibi kimi texnoloji parametrlərin müxtəlif qiymətləri üçün Si-Ge kristalında komponentlərin konsentrasiya profilləri hesablanmış və müzakirə edilmişdir. Ərinmiş zolağın uzunluğundan asılı olaraq tam dəyişən tərkibli kristallardan təxminən bircinsli materialın alınma imkanı göstərilmişdir. Alınan nəticələr Si-Ge kristallarının alınması üçün optimal şəraiti müəyyən edir.

Г.Х. Аждаров, А. Варилчи, Т. Кичикомероглу, М. Алтунбаш, А.И.Кобиа

РАСПРЕДЕЛЕНИЕ КОМПОНЕНТОВ В КРИСТАЛЛАХ Si-Ge, ВЫРАЩЕННЫХ МЕТОДОМ ЗОННОЙ ПЛАВКИ

Проведён анализ распределения компонентов в массивных кристаллах Si-Ge, выращенных методом зонной плавки, с целью определения операционных параметров для выращивания материала с заданным однородным и/или переменным концентрационным профилями. Рассчитаны и обсуждены концентрационные профили компонентов в кристаллах Si-Ge для ряда значений операционных параметров, таких как длина расплавленной зоны и исходный состав материала. Установлено, что концентрационный профиль Si, вдоль оси кристаллизации слитка Si-Ge, как функция длины расплавленной зоны изменяется значительно от полностью переменного до почти однородного. Полученные результаты определяют оптимальные операционные параметры для выращивания твердых растворов Si-Ge.

Дата поступления: 14.03.01

Редактор: М.И. Алиев