# THE DISTRIBUTION OF INDIUM IMPURITY IN THE Ge-SI HOMOGENEOUS CRYSTALS OF THE SOLID SOLUTIONS, GROWN UP BY BRIDGMAN METHOD IN THE MODE OF THE CONTINUOUS REPLENISHMENT OF THE MELT BY THE SILICON

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The problem of the distribution of the indium impurity in the homogeneous single crystals Ge-Si, grown up by Bridgman method with the use of the fuse and feeding ingot of the silicon has been solved in Pfann approximation. The concentrational profiles of the indium impurity along the crystallization axis of ingots with the different compositions, demonstrating the considerable influence of the change of the melt volume on these characteristics, connected with replenishment of the melt and dependence of the segregation coefficient of the impurity on the crystal composition.

The actuality of the investigations, directed on the study of the impurity centers in the semiconductors is defined by the fact, that work of the numerous devices, lying in the base of the modern micro-optoelectronics, is defined in many cases by the impurities of the different types, introduced into the crystal. The indium is the one of the most usable impurity for the doping of the crystals of the silicon, germanium and their solid solutions. Because of the big enough solubility and small activation energy the indium impurity defines the electronic properties of these semiconductors in the wide interval of the temperatures [1,2]. The balanced segregation coefficient of indium impurity is K<sub>In</sub>=0,0004 in Si and  $K_{In} = 0,001$  in Ge at the melting temperature of the silicon and germanium [3-5]. The small values of  $K_{In}$  in Si and Ge lead to the significant axial gradient of the impurity gradient in the semiconductor, grown up from the melt by the traditional methods of Bridgman or Chokhralsky. The questions, connected with the regularities of the distribution of the impurity centers in the simple semiconductors, doped in the process of the growing up from the melt, have been solved in the different approximations enough totally [1,4].



*Fig.1.* The schematic image of the growth of the homogeneous Ge-Si single crystal with indium impurity by the modernized Bridgman method.

The aim of the present paper is the solution of the task of the distribution of the indium impurity in the homogeneous crystals of the solid solutions Ge-Si, grown up by the modernized method of Bridgman in the mode of the constant replenishment of the melt by the silicon with taking under the consideration of the dependence of the distribution coefficient on the composition of the growing crystal. The task was solving in Pfann approximation and in the frameworks of the model of the virtual crystal for the solid solutions.

The scheme put in the base of the mathematic modeling of the concentration profile of the indium impurity in Ge-Si ingot, grown up in the mode, supplying the homogeneity of the distribution of the matrix atoms in the crystals is given on the fig.1. Initially, the feeding rod of silicon is contacted with the melt surface after the melting of the charging under the fuse from Ge, Si and In impurities with the corresponding ratio of the components and establishment of the temperature of the liquids of the given composition. Further, when the stabilized time is up, the mechanisms of the crystal drawing out and putting of the replenishment in the melt are engaged simultaneously. The growth of the homogeneous crystal with the given ratio of the concentrations of Ge and Si atoms is carried out by the way of the maintenance of the achieved temperature on the crystallization front because of the balancing of the melt composition by the corresponding ratio of the velocities of its crystallization and feeding. In this case the following ratio is correct [6-8]:

$$C_l^{Si} = \frac{\alpha}{K_{Si} - 1 + \alpha} \quad \text{or} \quad C_c^{Si} = \frac{K_{Si}\alpha}{K_{Si} - 1 + \alpha} \quad (1)$$

Here  $C_l^{Si}$  and  $C_c^{Si}$  are concentrations of the silicon in the melt and growing up homogeneous crystal correspondingly;  $\alpha$  is the ratio of the volume of the feeding of the ingot of the silicon, entered into melt to the volume of the crystallizing melt in time unit;  $K_{Si}$  is segregation coefficient of silicon in the given composition. The equation (1) gives the possibility to define the value of  $\alpha$  for any given  $C_l^{Si}$  or  $C_c^{Si}$ . Moreover, the corresponding value of  $K_{Si}$  is calculated from the phase diagram of the system state Ge-Si [1]. The dependence  $K_{Si}$  on the composition of the growing crystal, calculated by such way, is presented on the fig.2.

The task of the distribution of the indium impurity in Ge-Si crystals was solved under the following conditions: the crystallization front is plane; the equilibrium between solid and liquid phases exists on the crystallization front; the diffusion of indium impurity and convection in the melt supply the homogeneity of the liquid phase on all volume; the diffusion of the impurity atoms in the solid phase is approximately small. It is noted, that these conditions are realized at the growth velocities of crystal, which are less than  $1 \times 10^{-6}$  m/c [6].



*Fig.2.* The dependence of the equilibrium segregation coefficient of silicon on the composition of the solid phase of Ge-Si system, calculated from phase state diagram [1].

Let's introduce the following designations:  $V_l^0$ ,  $V_l$  are volumes of the melt in the crucible in the initial and current moments of time;  $V_c$ ,  $V_{Si}$  are the volumes of the crystallizing melt and dissolving silicon rod in time unit;  $C_{In,l}^0$ ,  $C_{In,l}$  are concentrations of indium impurities in the melt in the initial and current moments on time;  $C_{In,s}$  is concentration of indium impurities in the solid phase; *C* is common quantity of indium atoms in the melt;  $K_{In} = C_{In,s} / C_{In,l}$  is equilibrium segregation coefficient of indium; *t* is time.

We have with the above mentioned designations:

$$C_{In,l} = \frac{C}{V_l} \text{ and } \frac{dC_{In,l}}{dt} = \frac{\dot{C}V_l - \dot{V}_l C}{V_l^2} = \frac{\dot{C}V_l C}{V_l}.$$
 (2)

Taking into the consideration, that  $V_c$  and  $V_{Si}$  don't depend on time in the considerable period, we have:

$$V_{l} = V_{l}^{0} - (V_{c} - V_{Si})t,$$
  

$$\dot{V}_{l} = -V_{c} + V_{Si} \text{ and } \dot{C} = -V_{c}C_{In,l}K_{In}.$$
(3)

Substituting the data (2) in (1), after the separation of variables and integration, we find

$$\frac{V_c - V_{Si}}{V_c - V_c K_{Al} - V_{Si}} \int_{C_{In,l}^o}^{C_{In,l}} \frac{dC_{In,l}}{C_{In,l}} = \int_0^t \frac{\frac{dt(V_c - V_{Si})}{V_l^0}}{1 - \frac{(V_c - V_t)t}{V_l^0}}.$$
 (4)

Introducing designations  $V_{Si}/V_c = \alpha$ ;  $V_c t/V_l^0 = \gamma$ in (3) after integration, we obtain:

$$C_{In,s} = C_{In,l} K_{In} = C_{In,l}^{0} K_{In} \left[ 1 - \gamma (1 - \alpha) \right]^{\frac{(K_{In} + \alpha - 1)}{(1 - \alpha)}}.$$
 (5)

The equation (5) gives possibility to define the concentration of indium impurity in the dependence on  $\gamma$ , i.e. on crystal length at the known values  $K_{ln}$  and  $\alpha$ . The [1]

coefficient of the separation of  $K_{ln}$  impurity in Ge-Si crystal with given composition can be defined in the limits of the model of virtual crystal for the solid solutions on the known data  $K_{ln}$  in germanium and silicon, taking under the consideration, that  $K_{ln}$  depends linearly on the silicon concentration in the crystal. The experimental data of the ref [3] on the definition  $K_{ln}$  in the one of the compositions Ge-Si prove the correctness of the mentioned by us approximation. The value  $V_{Si}/V_c = \alpha$ ; in the equation (5), is defined from the condition of the growth totally homogeneous crystals of the solid solutions Ge-Si with the help of the equation (1).

The fig.3 illustrates the calculated curves of the concentration profile of indium impurity along Ge-Si crystals with silicon content 5, 10, 20, 40 and 80 at.% Si, calculated from the equation (5) with the use of the corresponding values  $\alpha$  and  $K_{Si}$  on data (1) and fig.2. For all crystals the initial concentration of the impurity in the melt is equal to  $C_{ln\,l}^0 = 1 \times 10^{18} \text{ cm}^{-3}$ .



*Fig.3.* The dependences of the concentration of the indium impurity on  $\gamma$  in homogeneous Ge-Si crystals, grown up by modernized Bridgman method with the use of the feeding silicon ingot. The curves 1, 2, 3, 4 and 5 are related to the crystals with the silicon content 5, 10, 20, 40 and 80 at.% correspondingly.

As it is seen from the fig.3, the velocity of the concentration growth of the impurity on the crystal length decreases with the increase of the silicon content in matrix. Such behavior is explained by the decrease of the segregation coefficient of indium with increase of silicon concentration in melt from one side, and with the increase of the melt volume, caused by its constant feeding from another side. It is need to pay attention on the practical constant of impurity concentration in enough extensive region in melts with big content of silicon. Such distribution character opens the possibility of the Ge-Si crystal obtaining with practically equal concentrational profile of indium impurity.

On the base of the above mentioned material, it is possible to make following conclusion. The dependence of segregation coefficient of the impurity on Ge-Si composition and change of the melt volume, connected with its feeding significantly influences on the velocity change of the concentration of the indium impurity along crystallization axis in homogeneous single crystals of the solid solutions Ge-Si, grown up by Bridgman method on the fuse with the given composition in the mode of the constant feeding of the melt by the second component.

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- [2] *V.M. Glazov, V.S. Zemskov*, Physico-khimicheskie osnovi legirovaniya poluprovodnikov, M.: Nauka, (1967) 371.
- [3] *B.I. Shklovskiy, A.L. Efros.* Elektronnie svoistva legirovannikh poluprovodnikov, M.: Nauka, (1979) 416.
- [4] Barz, P. Dold, U. Kerat, S. Recha, and K.W. Benz, Journal of Vac. Sci. Technol. B 16(3) (1998) 1627.
- [5] *D.T.J. Hurle*, Handbook of Crystal Growth (North-Holland, Amsterdam, 1994), vol.2b.
- [6] *M. Schulz and H. Weiss*, Landolt-Bornstein, New Series (Springer, Berlin) 1984.
- [7] G.Kh. Azhdarov, T. Kucukomerogly, A. Varilci, M. Altunbas, A. Kobya, P. G. Azhdarov. Journal of Crystal Growth, 226 (2001) 437.
- [8] *G.Kh. Ajdarov.* Izvestiya VUZov Rossii, Materiali elektronnoy tekhniki, 2 (2004) 47.
- [9] G.Kh. Ajdarov, R.Z. Kyazimzade, Tezisi dok. Natsionalnoy konferensii po rostu kristallov, Moskva (2004) c. 109.

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### SI-LA KƏSİRSİZ QİDALANAN ƏRİNTİDƏN MODERNLƏŞMİŞ BRİDJMAN ÜSULU İLƏ ALINAN BİRCİNSLİ Ge-SI KRİSTALLARINDA İNDİUM AŞQARININ PAYLANMASI

Pfann yaxınlaşması çərçivəsində modernizə edilmiş Bridjman üsulu ilə ərintini kəsirsiz Si ilə qidalandırma rejimində alınan bircinsli Ge-Si kristallarında indium aşqarının paylanma məsələsi nəzəri həll edilib. Aşqarın seqreqasiya əmsalının Ge-Si kristalının tərkibindən asılılığı və ərintinin qidalandırma nəticəsində dəyişilən həcmi aşqarın kristal boyunca konsentrasiyasına əhəmiyyətli təsiri göstərilib.

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#### РАСПРЕДЕЛЕНИЕ ПРИМЕСИ ИНДИЯ В ОДНОРОДНЫХ КРИСТАЛЛАХ ТВЁРДЫХ РАСТВОРОВ Ge-Si, ВЫРАЩЕННЫХ МЕТОДОМ БРИЖДМЕНА В РЕЖИМЕ НЕПРЕРЫВНОЙ ПОДПИТКИ РАСПЛАВА КРЕМНИЕМ

В пфанновском приближении решена задача распределения примеси индия в однородных монокристаллах Ge-Si, выращенных методом Бриджмена с использованием затравки и подпитывающего слитка кремния. Построены концентрационные профили примеси индия вдоль оси кристаллизации слитков различного состава, демонстрирующие существенное влияние на эти характеристики изменения объёма расплава, связанного с его подпиткой и зависимости коэффициента сегрегации примеси от композиции кристалла.

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