DISTRIBUTION OF THE COMPONENTS IN THE CRYSTAL Si-Ge, WHICH HAS BEEN BROUGHT UP BY THE DOUBLE FEEDING OF THE MELT METHOD

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A problem of component distribution in Si -Ge crystals grown under the continuous feeding of the melt with Silicon and Germanium rods has been solved in consideration of the Pfann approximation. A composition of the single crystal as a function of the rations of the crystallization and feeding rates of the melt as well as the melt composition is established. A possibility in preparing Si-Ge bulk single crystals with a desired uniform and compositionally graded profiles is shown.

The scientific and practical interest to the semiconductor solid solutions is defined mainly by the possibility of the precision control of their forbidden band width, parameters of the crystal structure and electric properties by the way of the corresponding change of the crystal composition. It is known, that classic semiconductors Si and Ge, being in the base of the modern electronics, dissolve in each other at any ratios as in the liquid, so in the solid states completely [1]. The questions, corresponded with the distribution of components in the volume crystals Si-Ge, which has been brought up from the melt by the different methods, were considered in many refs [2-7]. In ref [2] the good agreement of the experimental and calculation dates are established on the distribution of components in crystal Si-Ge, which have been brought up by Chohral method and feeding of the melt by the second component (Si) method.

In the present paper the problem of the distribution of components in the crystals Si-Ge, which have been brought up by Chohral method at the continuous double feeding of the melt by the composite components (Si and Ge) is solved. The aim of this investigation is the establishment of the operational parameters and conditions for the bringing up of the crystals Si-Ge with the given distribution of the components along the axis of the crystallization, including the homogeneous distribution.

The essence of the method of the double feeding of the melt is as follows: from the moment of beginning of the single crystal growth from corresponding melt the rods from composite components are introduced in it. During of the all cycle of the growth the crystallization velocity and velocity of the feeding of the melt by the first and second components are maintained constant.

The task was solved in the Pfann approximation at the satisfaction of the following standard conditions [2]: the crystallization front is plane; the balance, which is defined by the phase diagram between solid and liquid phases, is on the crystallization front; the diffusion of the atoms Si and Ge is the scornly small; the diffusion velocities of the atoms of the composite components in the melt are high enough and that's why the uniformity of melt composition is provided on the all volume.

We note that all these conditions in the system Si-Ge satisfy practically at the crystal velocity of growth <5mm/h [2,3,7].

Let's introduce the following designations V_m^o and V_m are melt volumes in the tigel at the initial and current moments; V_c is the melt volume crystallized in the unite of time; V_{Ge} and V_{Si} are volumes of the feeding ingots of the Ge and Si, introducing into the melt in the unite of time; C_{2m} and C_{2c} are concentrations of the second component atoms (Ge or Si) in the melt and crystal correspondingly; C is the general quantity of the second component in the melt; $K=C_{2c}/C_{2m}$ is the equilibrium segregation coefficient of the second component; t is time. Taking into consideration the above mentioned designations, we have:

$$C_{2m}=\frac{C}{V_m} \text{ and } \frac{dC_{2m}}{dt}=\frac{\dot{C}V_m-\dot{V}C}{V_m^2}=\frac{\dot{C}-\dot{V}_m C_{2m}}{V_m} \qquad (1)$$

On the task consideration we propose that V_c, V_{Ge} and V_{Si} don't depend on time. In this case the following equation takes place:

$$V_m=V_m^0 -(V_c-V_{Ge}-V_{Si})t \quad , \quad \dot{V}_m=-V_c+(V_{Ge}+V_{Si}),$$
$$\dot{C}=-V_c C_m K+V_2 \qquad (2)$$

Substituting the equation (2) into equation (1) we obtain:

$$\frac{dC_{2m}}{dt}=\frac{-V_c C_{2m}K+V_{Si}+V_c C_{2m}-(V_{Si}+V_{Ge})C_{2m}}{V_m^0-(V_c-V_{Si}-V_{Ge})t} \qquad (3)$$

After the variables' separation in the equation (3) and integration, we have:

$$\frac{V_c K-V_c+V_{Si}+V_{Ge}}{V_c-V_{Si}-V_{Ge}} ln\frac{V_m^0}{V_m^0-(V_c V_{Si}-V_{Ge})t}=ln\frac{V_{Si}-(V_c K-V_c+V_{Si}+V_{Ge})C_{2m}^0}{V_{Si}-(V_c K-V_c+V_{Si}+V_{Ge})C_{2m}} \qquad (4)$$

In the equation (4) the integration constant is defined from the initial condition $C_{2m}=C^0_{2m}$ at $t=0$. Let's introduce the following equations: $\gamma=V_c t/V^0_m$, $\alpha=V_{Si}/V_c$, $\beta=V_{Ge}/V_c$ and with the help of them from the equation (4) after the uncompound transformations, we obtain:

$$C_{2c}=C_{2m}K=\frac{K}{K-1+\alpha+\beta}\left\{\alpha-\left[\alpha-(K-1+\alpha+\beta)C^0_{2m}\right]\times\left[1-(1-\alpha-\beta)\gamma\right]^{\frac{K-1+\alpha+\beta}{1-\alpha-\beta}}\right\} \quad (5)$$

For the special case, when $\alpha+\beta=1$ it is obviously that $V_m=V^0_m$ and $V_m=0$. Then from the equation (1) after the several transformations we obtain:

$$C_{2c}=\alpha-(\alpha-KC^0_{2m})e^{-\gamma K} \quad (6)$$

The formulas (5,6) give the distribution of the second component on the crystal length l (as $\gamma\sim l$) in dependence on the operational parameters α, β and C^0_{2m}.

The one of the widespread variants for the single crystals obtaining of the solid solutions Si-Ge by the feeding of the melt method is the using of the pure main component (Si or Ge) in the capacity of the initial melt [2]. Using of this variant is connected with the difficulty of the obtaining of the seedings with the different concentrations of atoms Si and Ge, corresponding with the initial melt composition. For this variant, when $C^0_{2m}=0$, from the equations (5) and (6) correspondingly we obtain:

$$C_{2c}=\frac{K\alpha}{K-1+\alpha+\beta}\left\{1-\left[1-(1-\alpha-\beta)\gamma\right]^{\frac{K-1+\alpha+\beta}{1-\alpha-\beta}}\right\} \quad (7)$$

$$C_{2c}=\alpha(1-e^{-\gamma K}) \quad (8)$$

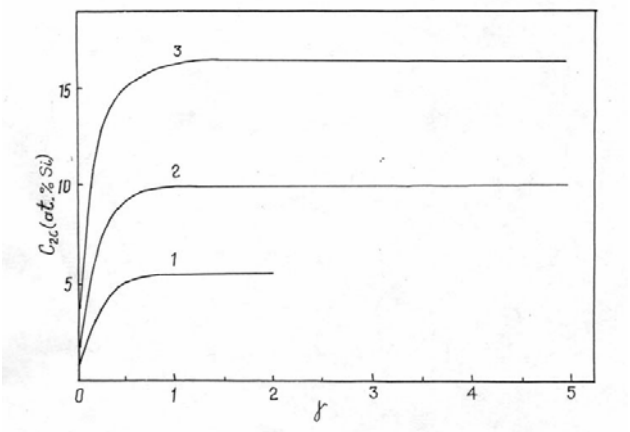

Fig.1. Dependences of concentration of the second component with $K>1$(Si) on γ for crystals Si-Ge, constructed on the base of the expressions (7) (curves 1, 3) and (8) (curve 2).

In the figure 1 for example the dependence curves of the second component-Si in the crystal Ge-Si on γ for the three different values $\alpha+\beta$, which are equal to 0,5, 1 and 2, calculated from the equations (7) and (8) are given. In all cases it is noted that $\alpha:\beta$=1:9, that corresponds with the feeding of the melt by the solid solution with 10 at.%Si. The Si segregation coefficient is equal to equilibrium one, which is defined from the phase diagram (K=5.5 [8]). The initial material of the melt in the tigel is Ge. The analogous calculated curves, for the case when the second component is Ge with K=0,33 [8], are given in the fig. 2. Here the initial material of the melt in the tigel is Si. The curves 2 in the figures correspond with the case, when $\alpha+\beta=1$ and are constructed on the base of the equation (8). If for $\alpha+\beta=1$ the process of the crystal growth can be continued unlimited (curves2 and 3), then for $\alpha+\beta<1$ this process is limited by the melt in tigel (curve1). This corresponds with the expression in the square bracket in the equation (7) is equal to zero. Indeed, if $t=t_{max}$, the term $[1-(1-\alpha-\beta)\gamma]=0$, then $V_m=V^0_m-(V_c-V_{Ge}-V_{Si})t=0$. Practically, of course, the single crystal growth ends earlier, than at $t=t_{max}$. The analysis of the equations (5-8) and given for the example curves' stroke (fig.1) show that at $K>1$ for any remain constant values α, β one can obtain the single crystal with the practically homogeneous composition. In addition, the part of the second component in the homogeneous part of the crystal is defined by the multiplier before the brace in the equation (5) or (7) for the cases, when $\alpha+\beta\neq1$ and is equal α at $\alpha+\beta=1$. The variant, when the second component is Ge with $K<1$ (fig.2), its concentration grows continuously on the crystal length at $\alpha+\beta<1$ (curve 1) and that's why this case can be applied only for the obtaining of the crystals with the variable composition. At $\alpha+\beta=1$ correspondingly with the equations (5-8) and dates of fig.2, in principle the single crystal with the uniform distribution of components can be obtained, but it is no need to apply this method in practically because of the big enough length of the inhomogeneous region (curves 2 and 3). Obviously, that single-minded calculations, carried out for the different values α, β and $\alpha+\beta$, will define the operational parameters for the bringing up of the crystals Si-Ge with the given distribution of components.

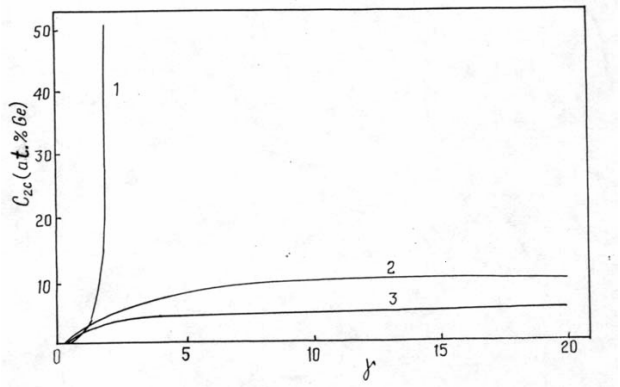

Fig.2. Dependences of concentration of the second component with $K<1$(Ge) on γ for crystals Si-Ge, constructed on the base of the expressions (7) (curves1,3) and (8) (curve 2).

The practical realization of the double feeding of the melt method for the bringing up of the single crystals Si-Ge can be done on the installation, described in the ref [9], which has the automatic system for the supporting of the given diameter

of the growing crystal and the input mechanism of the feeding ingots in the melt. The pulling velocity of the single crystal Si-Ge should be within 1-5mm/h for the carrying out of the criterion of the equilibrium state between crystal and melt [2,3,10].

On the base of the above mentioned we can do the following conclusion. The problem solving of the distribution of components in the crystals SiGe, brought up by the double feeding of the melt method in Pfann approximation, shows the possibility of the obtaining of the single crystals as with variable, so with the homogeneous compositions. The obtained expressions allow to find the optimal conditions of the crystal growth with the given distribution of components.

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ƏRİNTİNİ İKİQAT QİDALANDIRMA ÜSULU İLƏ ALINAN Si-Ge KRİSTALLARINDA KOMPONENTLƏRİN PAYLANMASI

Silisium və germanium ilə fasiləsiz qidalanan ərintidən yetişdirilən Si-Ge kristallarında komponentlərin paylanma məsələsi Pfann yaxınlaşmasında həll edilib. Yetişdirilən monokristalın tərkibinin ərintinin kristallaşma və qidalanma sürətlərinin münasibətindən və onun başlanğıc konsentrasiyasından asılılıq tənlikləri alınıb. Si-Ge monokristallarında verilmiş dəyişən və bircinsli komponent paylanması əldə etmək imkanı göstərilib.

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РАСПРЕДЕЛЕНИЕ КОМПОНЕНТОВ В КРИСТАЛЛАХ Si-Ge, ВЫРАЩЕННЫХ МЕТОДОМ ДВОЙНОЙ ПОДПИТКИ РАСПЛАВА

В пфанновском приближении решена задача распределения компонентов в кристаллах Si-Ge, выращенных в условиях непрерывной подпитки расплава кремниевым и германиевым стержнями. Получены уравнения, определяющие композицию растущего монокристалла в зависимости от соотношения скоростей кристаллизации и подпитывания расплава, а также стартового состава расплава. Показана возможность получения монокристаллов Si-Ge с заданными переменными и однородными составами.

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