SIMULATION OF THE FORMATION OF PRIMARY GROWN-IN MICRODEFECTS IN DISLOCATION-FREE SILICON SINGLE CRYSTALS

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A mathematical model of the formation of primary grown-in microdefects on the base of the dissociation diffusion process is presented. The cases of the interactions "oxygen-vacancy" (V+O) and "carbon-self-interstitials" (C+I) near the crystallization front for dislocation-free silicon single crystals, which were obtained by the floating zone and Czochralski methods, are considered. The obtained approximate analytic expressions correlate with the heterogeneous mechanism of the formation of grown-in microdefects.

1. Introduction

Grown-in microdefects determine not only the initial defective structure of dislocation-free silicon monocrystals, but also a subsequent transformation of this structure during the technological processing. Therefore, the study of the mechanism of of the formation of grown-in microdefects is a key to solve the problem of the control over a crystal defective structure and to understand the fundamental interactions of point-like defects.

Now there are two approaches in solving the problem of the formation of grown-in microdefects. The authors of the first approach work within the framework of a model of the dynamics of point defects, in which the crystal is considered as a dynamical system or solid-state chemical reactor, where the transition and interaction of point defects occur. It is supposed that the modeling of the dynamics of point defects gives the quantitative understanding of the formation of grown-in microdefects and their space distribution [1]. The model of the dynamics of point defects includes a convection, diffusion, and recombination of intrinsic point defects. In this model, the critical role is played by the process of fast recombination of intrinsic point defects near the melting temperature. All modifications of this model of the dynamics of point defects are based on the Voronkov theoretical model of the formation of grown-in microdefects [2], where it was assumed that 1) the recombination rate of intrinsic point defects near the melting temperature is very high, 2) the diffusivities of self-interstitials near the melting temperature are greater than those of vacancies, 3) the equilibrium concentration of vacancies near the melting temperature is more than the equilibrium concentration of self-interstitials. Voronkov showed that the formation of grown-in microdefects is controlled by the critical growth parameter $V/G = C_{\mathrm{crit}}$ (where V is the crystal growth rate, and G is the axial temperature gradient). This theoretical model describes the formation of vacancy microvoids (the agglomeration of vacancies) at $V/G > C_{\mathrm{crit}}$ and interstitial dislocation loops at $V/G < C_{\mathrm{crit}}$ in various areas of a crystal. From our viewpoint, despite the subsequent updating [3], an essential defect of the Voronkov model is the weak point of the interaction between impurities and intrinsic point defects.

The second approach is experimental researches of the physical nature and characteristics of grown-in microdefects [4]. On the base of these researches, we have developed the qualitative heterogeneous mechanism of the formation and transformation of grown-in microdefects which is based on the following positions [5]:

— recombination of intrinsic point defects near the melting temperature is insignificant because of the availability of a recombinational barrier;

— disintegration of the oversaturated solid solution of intrinsic point defects during the crystal cooling passes by two mechanisms: the vacancy and interstitial ones;

— background impurities of oxygen and carbon take the direct participation in the formation of grown-in microdefects and the transformation process.

It is clear that the main principles of the heterogeneous mechanism contradict the theoretical positions of the Voronkov model. Therefore, we consider that the main defect of the heterogeneous mechanism is the absence of an appropriate mathematical model. The purpose of this paper is the substantiation of a theoretical model of the heterogeneous mechanism of

the formation of grown-in microdefects as a result of the interaction "impurity — intrinsic point defect".

2. Physical Model

We have shown that the defect formation process involves oxygen-vacancy and carbon-interstitials agglomerates which are formed at impurities centers [5]. It was experimentally established that the formation of oxygen-vacancy and carbon-interstitial agglomerates ($(I + V)$-microdefects) begins close to the melting temperature [4]. It is known that secondary grown-in microdefects are formed at a crystal cooling for temperatures below 1200 °C [6]. Based on this experimental results, we offered the concepts of primary grown-in microdefects ($(I + V)$-microdefects, $D(C)$-microdefects, B-microdefects), and secondary grown-in microdefects (A-microdefects, vacancy microvoids). These concepts are based on the following interaction types: the primary (fundamental) "impurity — intrinsic point defects" and secondary ("intrinsic point defects — intrinsic point defects") interactions, respectively.

We offer to consider a crystal defective structure as a structure which consists of two subsystems: the subsystem of primary grown-in microdefects and the subsystem of secondary grown-in microdefects. The subsystem of secondary defects (vacancy microvoids and interstitial dislocation loops) can be described by the Voronkov theoretical model. In this paper, we consider the formation of primary grown-in microdefects.

As was mentioned above, in dislocation-free silicon single crystals which were grown by the floating zone method (FZ-Si) and the Czochralski method (Cz-Si), the recombination of intrinsic point defects close to the crystallization front is insignificant because of the availability of an entropy recombinational barrier [4, 6]. As for temperatures close to the melting temperature, there are simultaneously the equilibrium concentrations of vacancies and self-interstitials, and the disintegration of the oversaturated solid solution of point defects happens simultaneously by two mechanisms. In the correspondence with the sign of the silicon crystalline lattice strain, these mechanisms were called the vacancy and interstitial ones. Based on the heterogeneous mechanism of the formation of grown-in microdefects, the vacancies (V) and self-interstitials (I) find drains in the form of background impurities of oxygen (O) and carbon (C), respectively. At the initial defect formation stage, these processes result in the formation of complexes (V+O) and (C+I). It is possible to write the following quasichemical equation:

a) for the vacancy path of the heterogeneous mechanism — $\mathrm{O}_i + V \rightarrow (\mathrm{O}+V)$

b) for the interstitial path of the heterogeneous mechanism — $\mathrm{C}_S + I \rightarrow (\mathrm{C}+I)$,

where O_i — interstitial oxygen atoms, and C_S — subsequent carbon atoms.

Such idealized system is typical of non-doped monocrystals FZ-Si which are grown in vacuum with a concentration of oxygen and carbon less than 5×10^{15} cm^{-3}. It is necessary to consider that this system does not take into account a possibility of the joint interaction of O_i and C_S. Furthermore, in real crystals FZ-Si and Cz-Si, it is necessary to take into account the availability and interaction of other point defects (e.g., iron, nitrogen, doped impurities).

In the present paper, we consider the idealized system for four variables (vacancy, self-interstitials, oxygen, carbon).

3. Mathematical Model

We are looking for the solution we search within the framework of a model of the dissociation diffusion-migration of impurities [7]. In this case, the difference from the process of disintegration is the following. In the diffusion, as a technological process, a diffusant arrives in a sample from an external source. But, during the disintegration, the diffusant arrives from an internal source, i.e. from sites of a crystalline lattice. The theoretical analysis is identical. However, for the determination of the dissociative diffusion, it is necessary to take into account the surface concentration which decreases in the volume of a sample in time along a coordinate. The time constant is determined by the mechanism of migration in the volume of a sample, and the dependence on a coordinate is determined by the form of a sample and the boundary conditions of the diffusion problem.

The interpretation of the diffusion in multicomponent systems is hampered by the necessity to account the interaction of the atoms of impurities. Generally, it is necessary to use the numerical methods of solving the equations, and it is possible to obtain simple analytical expressions which are convenient for a comparison with experiment only in the certain approximations. The mechanism of the formation of complexes can be different but irrespective of the nature of forces which result in the nucleation of complexes. Any model assumes that the radius of these forces should be small. In this case, in the analysis of the migration of

point defects, the complex can be considered as a point defect.

Let's consider the formation of complexes as a quasichemical reaction

$$A + B \leftrightarrow AB. \tag{1}$$

Then the condition of a thermodynamic equilibrium between free impurity A and impurity B which are joined in complex AB will be written as

$$\mu_{\rm A} + \mu_{\rm B} = \mu_{\rm AB}, \tag{2}$$

where $\mu_{\rm A}$ and $\mu_{\rm B}$ are the chemical potential of free impurities, and $\mu_{\rm AB}$ is the chemical potential of the complex.

If the full concentration of impurities A and B ($N_{\rm A}$, $N_{\rm B}$) is small in comparison with the concentration of the main component, then, in this approximation, $\mu_{\rm AB} \approx \ln N_{AB}$, and the equilibrium condition (2) can be presented as

$$\frac{(N_{\rm A} - Q)(N_{\rm B} - Q)}{Q} = k(T). \tag{3}$$

Here, Q is the concentration of complexes, $k(T)$ is the rate constant of the formation of complexes which depends on temperature (at a constant pressure) [8]. At $k = 0$, all impurities are bound in complexes (the force formation of complexes).

With regard for the formation of complexes, the full diffusion flow of impurities consists of the flows of free impurities and impurities included in complexes [8]:

$$\frac{\partial N_{\rm A}}{\partial t} = D_{\rm A}\frac{\partial^2 (N_{\rm A} - Q)}{\partial x^2} + D_Q\frac{\partial^2 Q}{\partial x^2}, \tag{4}$$

$$\frac{\partial N_{\rm B}}{\partial t} = D_{\rm B}\frac{\partial^2 (N_{\rm B} - Q)}{\partial x^2} + D_Q\frac{\partial^2 Q}{\partial x^x}, \tag{5}$$

where $N_{\rm A}$ and $N_{\rm B}$ are the impurity concentrations; $D_{\rm A}$, $D_{\rm B}$, and D_Q are the diffusivities of free components A and B and the diffusivities of complexes, respectively.

The diffusivity of complexes depends on the mechanism of the formation of complexes and on a type of components which form complexes. In particular, if the complex is formed by two interacting atoms, then the diffusivity D_Q is much less than $D_{\rm A}$ and $D_{\rm B}$. Therefore, by considering complexes to be poorly mobile, it is possible to neglect the last terms in Eqs. (4) and (5):

$$\frac{\partial N_{\rm A}}{\partial t} = D_{\rm A}\frac{\partial^2 (N_{\rm A} - Q)}{\partial x^2}, \tag{6}$$

$$\frac{\partial N_{\rm B}}{\partial t} = D_{\rm B}\frac{\partial^2 (N_{\rm B} - Q)}{\partial x^2}. \tag{7}$$

As the complexes do not move, the boundary conditions are those for free impurities. As the relaxation time to the equilibrium between complexes and free impurities is much more than the characteristic times of the diffusion, it is possible to take the full concentration of impurities as the initial conditions.

In [8], the problem of the sequential diffusion of component A in a sample which is homogeneously doped by component B was considered with taking the formation of complexes into account in the initial and boundary conditions:

$$N_{\rm A}(x,0) = 0,$$

$$N_{\rm B}(x,0) = N_{\rm B}(\infty),$$

$$N_{\rm A}(0,t) - Q(0,t) = H_{\rm A}(0),$$

$$\frac{\partial}{\partial x}[N_{\rm B}(x,t) - Q(x,t)]_{x=0} = 0. \tag{8}$$

Then the diffusion equation looks as

$$\left.\begin{aligned} &\frac{1}{2}\Big[N_{\rm A} - N_{\rm B} - k + (k^2 + 2k(N_{\rm A} + N_{\rm B}) + \\ &+(N_{\rm A} - N_{\rm B})^2)^{1/2}\Big]'' + 2\lambda N_A' = 0, \\ &\frac{1}{2}\Big[N_{\rm B} - N_{\rm A} - k + (k^2 + 2k(N_{\rm A} + N_{\rm B}) + \\ &+(N_{\rm A} - N_{\rm B})^2)^{1/2}\Big]'' + 2\lambda d^2 N_{\rm B}', \end{aligned}\right\} \tag{9}$$

where $\lambda = \frac{x}{2\sqrt{D_{\rm A}\cdot t}}$ is the Boltzmann substitution, the "prime" designates the derivative with respect to λ, $d^2 = \frac{D_{\rm A}}{D_{\rm B}}$, and $D_{\rm A}, D_{\rm B}$ are the diffusivities of components.

The solution of the system of equations (9) with appropriate boundary conditions (the diffusion of impurity A from a constant source in a semiconductor which is homogeneously doped by impurity B; impurity B does not evaporate) in the case of the force formation of complexes ($k = 0$) is as follows [8]:

$$N_{\rm A} = \begin{cases} N_{\rm B1} + H_{\rm A}(0)\Big[1 - \frac{\mathrm{erf}(\lambda/d_{\rm A})}{\mathrm{erf}(\lambda_0/d_{\rm A})}\Big], & \lambda < \lambda_0, \\ 0, \quad \lambda > \lambda_0, \end{cases} \tag{10}$$

$$N_{\mathrm{B}} = \begin{cases} N_{\mathrm{B1}}, & \lambda < \lambda_0, \\ N_{\mathrm{B0}}(1 - \frac{\mathrm{erf}c(\lambda d)}{\mathrm{erf}c(\lambda_0 d)}), & \lambda > \lambda_0, \end{cases} \tag{11}$$

where

$$N_{\mathrm{B1}} = \frac{N_{\mathrm{B0}} e^{-\lambda_0 d^2}}{\sqrt{\pi}\lambda_0 d \mathrm{erf}c(\lambda_0 d)}, \tag{12}$$

and λ_0 is determined from the equation

$$\frac{e^{\lambda_0^2(1-d^2)}\mathrm{erf}(\lambda_0)}{\mathrm{erf}c(\lambda_0 d)} = \frac{N_{\mathrm{A0}}}{N_{\mathrm{B0}}}. \tag{13}$$

Let's copy the system of equations (3)—(5) for the doping diffusion kinetics of mobile complexes in the language of full components $N_A = H_A + Q$ and $N_B = H_B + Q$:

$$d_{\mathrm{A}}^2(N_{\mathrm{A}} - Q)'' + d_Q^2 Q'' + 2\lambda N_{\mathrm{A}}' = 0, \tag{14}$$

$$d_{\mathrm{B}}^2(N_{\mathrm{B}} - Q)'' + d_Q^2 Q'' + 2\lambda N_{\mathrm{B}}' = 0, \tag{15}$$

$$(N_{\mathrm{A}} - Q)(N_{\mathrm{B}} - Q) = k(T)Q, \tag{16}$$

where $d_{\mathrm{A}}^2 = D_{\mathrm{A}}$; $d_{\mathrm{B}}^2 = D_{\mathrm{B}}$; $d_Q^2 = D_Q$; D_Q is the diffusivity of complexes; the "primes" mean the derivative with respect to λ.

Let's remark that the solution of the system of equations is considered for three cases which are most frequently met in practice: the sequential, simultaneous, and mutual diffusion. Under conditions of our physical model, it is possible to consider the sequential diffusion when, on the boundary of the unit, there is no flow of components which is set at the initial time in the volume of a sample. In this case, the boundary conditions look as

$$H_{\mathrm{A}}|_{\lambda=0} = H_{\mathrm{A}}(0); \quad H_{\mathrm{A}}|_{\lambda=\infty} = H_{\mathrm{A}}(\infty),$$

$$d_{\mathrm{B}}^2 H_{\mathrm{B}}' + d_Q^2 Q'|_{\lambda=0} = 0; \quad H_{\mathrm{B}}|_{\lambda=\infty} = H_{\mathrm{B}}(\infty). \tag{17}$$

Generally, the system of equations (14)—(16) with the boundary conditions (17) has no analytic solutions. Therefore, for the analysis of doping structures, it is necessary to consider the limiting cases. Let's consider the approximation of the force formation of complexes ($k = 0$). It means physically that the reaction A+B $\leftrightarrow Q$ is sharply shifted to the side of the complex formation. Furthermore, it follows formally from the system (14)—(16) at $k = 0$ that the concentration is equal to zero for at least one of the free components, i.e., $H_{\mathrm{A}} = 0$ or $H_{\mathrm{B}} = 0$ (the impurity is completely bound in complexes).

A solution of the diffusion equation for component A in a semi-infinite sample which is homogeneously doped by component B under condition of the absence of the evaporation of component B from a sample and the availability of free component A on the boundary of a sample has the form [7]

$$H_{\mathrm{A}} = N_{\mathrm{A}} - Q =$$

$$= \begin{cases} (N_{\mathrm{A}}(0) - N_{\mathrm{B1}})\left[1 - \frac{\mathrm{erf}c(\lambda/d_{\mathrm{A}})}{\mathrm{erf}c(\lambda_0/d_{\mathrm{A}})}\right], & \lambda \le \lambda_0, \\ 0, & \lambda > \lambda_0, \end{cases} \tag{18}$$

$$H_{\mathrm{B}} = N_{\mathrm{B}} - Q =$$

$$= \begin{cases} 0, & \lambda \le \lambda_0, \\ N_{\mathrm{B}}(\infty)\left[1 - \frac{\mathrm{erf}c(\lambda/d_{\mathrm{B}})}{\mathrm{erf}c(\lambda_0/d_{\mathrm{B}})}\right], & \lambda > \lambda_0, \end{cases} \tag{19}$$

$$Q = \begin{cases} N_{\mathrm{B1}}, & \lambda \ge \lambda_0, \\ N_{\mathrm{B1}}\frac{\mathrm{erf}c(\lambda/d_Q)}{\mathrm{erf}c(\lambda_0/d_Q)}, & \lambda < \lambda_0, \end{cases} \tag{20}$$

$$N_{\mathrm{B1}} T(\lambda_0/d_Q) = N_{\mathrm{B}}(\infty) T(\lambda_0/d_{\mathrm{B}}),$$

$$N_{\mathrm{B1}} T(\lambda_0/d_Q) = \{N_{\mathrm{A}}(0) - N_{\mathrm{B1}}\} S(\lambda_0/d_{\mathrm{A}}), \tag{21}$$

where

$$T(x) = \frac{\exp(-x^2)}{\sqrt{\pi}x\mathrm{erf}c(x)};$$

$$S(x) = \frac{\exp(-x^2)}{\sqrt{\pi}x\mathrm{erf}(x)}; N_{\mathrm{A}}(0) - N_{\mathrm{B1}} = H_{\mathrm{A}}(0).$$

4. Experimental

In our physical model (the heterogeneous mechanism of the formation of grown-in microdefects), it is accepted that component A is a background impurity (oxygen or carbon) and component B consists of intrinsic point defects (vacancies or self-interstitials). For the vacancy and interstitial mechanisms, we consider, respectively, the "oxygen + vacancy" interaction (O+V) and the "carbon + self-interstitials" one (C+I). In estimates, we used the following values:

$H_{\mathrm{A}}(0) = H_o(0) = 4 \times 10^{15}$ cm^{-3}(FZ-Si);

$H_{\rm A}(0) = H_o(0) = 8 \times 10^{16}$ cm^{-3}(Cz-Si);

$C_V = 8.84 \times 10^{14}$ cm^{-3};

$D_V = 4 \times 10^{-5}$ cm^2/s; $D_o = 0.17 \exp(-2.54/kT)$,

$k = 8.6153 \times 10^{-5}$ eV/k,

$H_{\rm A}(0) = H_c(T_m) = 4 \times 10^{15}$ cm^{-3}(FZ-Si),

$H_{\rm A}(0) = H_c(0) = 1 \times 10^{16}$ cm^{-3}(Cz-Si),

$C_I(0) = 6.31 \times 10^{14}$ cm^{-3}, $D_I = 4.75 \times 10^{-4}$ cm^2/s,

$D_c = 1.9 \exp(-3.1/kT)$.

The solution of Eqs. (12) and (13) has a physical sense ($N_{\rm B1} \sim 10^{12} \div 10^{14}$ cm^{-3}) only at $\lambda \approx 0.01$. Let's mark that, in the approximation of the force formation of complexes, λ_0 is interpreted as the boundary of the reaction front where complexes are formed. That is, let x be the crystal length, and let $x = 0$ be a position of the crystallization front. Then it is possible to say that the complex formation process happens close to the crystallization front.

These data are confirmed by experimental researches of initial stages of the defect formation process. We realized a quenching of non-doped monocrystals FZ-Si of 30 mm in diameter which were grown in vacuum at a various growth rates (2.0, 3.0, 6.0, 9.0 mm/min). We used one from the most effective methods of crystal quenching, namely the decantation of the melting zone, when the zone is sharply blown off by a directed argon flow at a certain instant. These experiments have allowed us to determine the temperatures of the formation of grown-in microdefects (see the Table) [4].

The quenching of FZ-Si grown at $V = 6$ mm/min results in the formation of the so-called "defect-free" area between the crystallization front and the area with D-microdefects. Transmission electronic microscopy (TEM) researches have shown that the "defect-free" area contains both of interstitial and vacancy defects with sizes 2 ... 7 nm and a concentration of $\sim 4.5 \times 10^{13}$ cm^{-3} ((I+V)-microdefects). In FZ-Si grown at $V = 9$ mm/min, we found interstitial and vacancy microdefects approximately in a comparable concentration after the quenching.

By studying the separation surface, we revealed that, at distances at most 1 ... 3 mm from the crystallization front, dislocations appear from a thermal impact. Therefore, it is inconvenient to precisely determine the beginning of the formation of primary grown-in microdefects. In view of the Table, we can conclude that primary grown-in microdefects are formed close to the crystallization front.

In Fig. 1*a,b*, we show $T(x)$ for FZ-Si (a diameter of 30 mm) and Cz-Si (a diameter of 50 mm). For FZ-Si, $T(x)$ was determined in correspondence with the empirical dependence [9]

$$\frac{dT}{d\ell} = 10 + (\ell - 16)^2 \exp(-61.2V - 0.28), \qquad (22)$$

where ℓ is the distance from the crystallization front to a considered cut, in cm, and V is the crystal growth rate, in cm/s.

For Cz-Si, it is accepted that $G_{\text{FZ-Si}} \approx 3G_{\text{Cz-Si}}$, where G is the axial temperature gradient. For FZ-Si and Cz-Si, we show the dependence at $V = 1 \ldots 9.0$ and 0.5 ... 3.0 mm/min, respectively. The radial temperature gradient was not taken into account; the distribution of defects in the crystal over a diameter is homogeneous.

The theoretical calculations were conducted for the vacancy (O+V) and interstitial (C+I) paths of the heterogeneous mechanism of the formation of grown-in microdefects in FZ-Si and Cz-Si. In Fig. 2*a,b*, we show $C_V/C_V(0), C_{Q1}/C_{Q1}(0)$ versus the Cz-Si crystal length in the range of growth rates 0.5 ... 3.0 mm/min (where $C_V(0)$ and $C_{Q1}(0)$ are the concentrations of vacancies and complexes (O+V) close to the crystallization front, respectively).

Temperatures of the formation of microdefects of various types

Growth rate, mm/min	Growth conditions	Microdefect type	Length from crystallization front, mm	Formation temperatures, ±2 K
2.0	quenching	*A*	23	$T_A = 1373$
3.0	quenching	*B*	—	$T_B = 1653$
6.0	quenching	*D*	26	$T_D = 1423$
6.0; 9.0	quenching	*I+V*	—	$T_{I+V} = 1653$

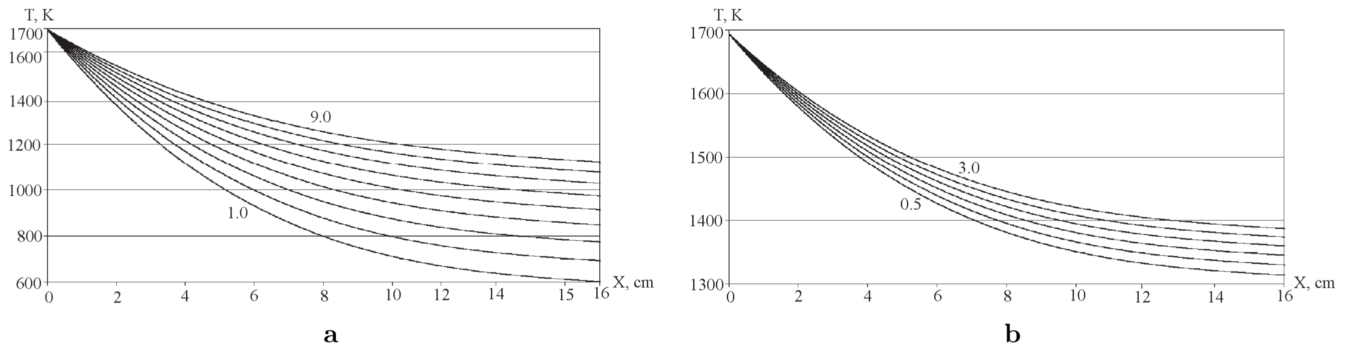

Fig. 1. Set of curves $T(x)$: (a) for FZ-Si grown at V = 1 ÷ 9.0 mm/min, (b) for Cz-Si grown at V = 0.5 ÷ 3.0 mm/min

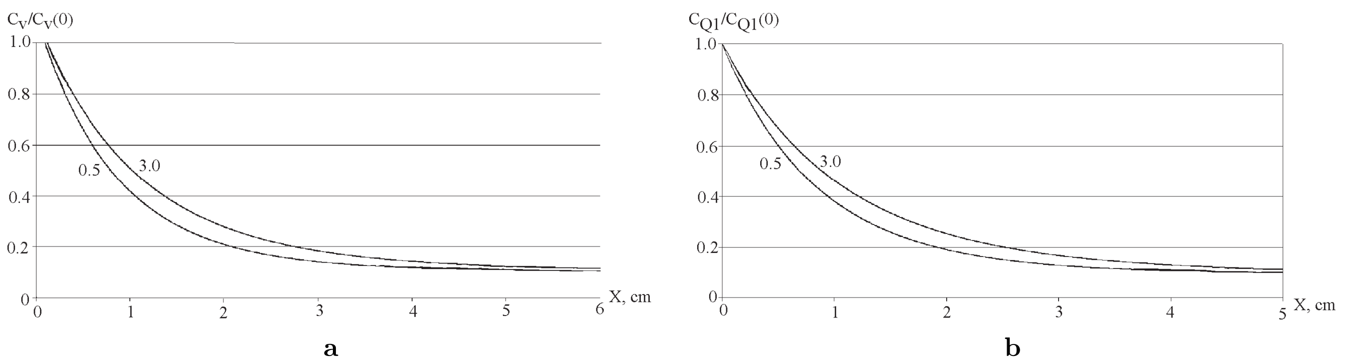

Fig. 2. Curves (a) $C_V/C_V(0)$, (b) $C_{Q1}/C_{Q1}(0)$ versus the crystal length for Cz-Si

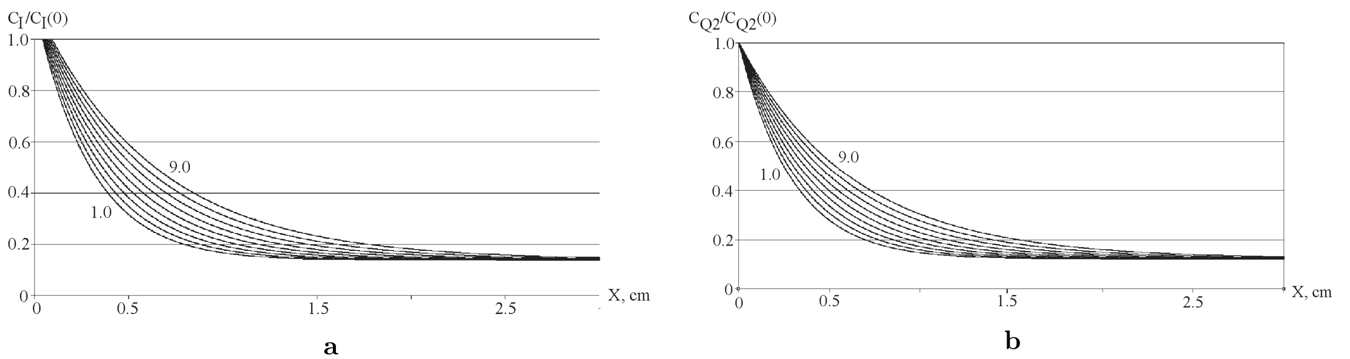

Fig. 3. Curves (a) $C_I/C_I(0)$,(b) $C_{Q2}/C_{Q2}(0)$ versus the crystal length for FZ-Si

Figure 3,*a,b* shows the calculated dependence $C_I/C_I(0), C_{Q2}/C_{Q2}(0)$ versus the FZ-Si crystal length in the range of growth rates 1—9.0 mm/min (where $C_I(0)$ and $C_{Q2}(0)$ are the concentrations of self-interstitials and complexes (C+I) close to the crystallization front, respectively). Indices 1 and 2 correspond to the vacancy and interstitial paths of the heterogeneous mechanism of the formation of grown-in microdefects, respectively.

The analysis of the calculated curves shows their good agreement with experimental data and the results of the heterogeneous mechanism of the formation of grown-in microdefects. This concerns the formation temperatures of primary grown-in microdefects, the experiments on the crystal quenching (Table), and the concentrations of $(I + V)$-microdefects and D (C)-microdefects determined in the TEM-researches ($\sim 10^{13} \div 10^{14}$ cm^{-3}) [4, 5]. Therefore, despite the

accepted assumptions, it is possible to conclude that the dissociative impurity diffusion model well agrees with the experimental results of studies of grown-in microdefects and can be a theoretical basis of the heterogeneous mechanism of the formation of grown-in microdefects. The formation of secondary grown-in microdefects (interstitial dislocation loops, vacancy microvoids) during the crystal cooling below 1200 °C can be stipulated by the transformation of an initial defective structure of primary grown-in microdefects [4] and the formation of the agglomerates of intrinsic point defects [5].

Furthermore, as distinct from the Voronkov model, there is a possibility to describe the fundamental properties of high purity crystals by the interaction of "impurity — intrinsic point defect". This will allow one, in turn, to create a uniform defect formation theory of dislocation-free silicon monocrystals in the future.

5. Conclusion

A mathematical model of the formation of primary grown-in microdefects based on the dissociation diffusion process is formulated for the first time. The cases of the interactions "oxygen-vacancy" (O+V) and "carbon-self-interstitials" (C+I) close to the crystallization front for dislocation-free silicon single crystals obtained by the floating zone and Czochralski methods are considered. The obtained approximate analytic expressions agree with the heterogeneous mechanism of the formation of grown-in microdefects.

This model has the following differences from the theoretical Voronkov model:
— it is completely based on experimental results instead of on the theoretical suppositions;
— it takes into account the interaction between impurity and intrinsic point defects;
— it allows one to adequately describe a microdefective structure of dislocation-free silicon monocrystals.

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МОДЕЛЮВАННЯ УТВОРЕННЯ
ПЕРВИННИХ РОСТОВИХ МІКРОДЕФЕКТІВ
У БЕЗДИСЛОКАЦІЙНИХ МОНОКРИСТАЛАХ КРЕМНІЮ

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Р е з ю м е

Запропоновано математичну модель процесу утворення первинних ростових мікродефектів, що ґрунтується на дисоціативному процесі дифузії. Розглянуто випадки взаємодії кисень—вакансія (V+O) і вуглець — власний міжвузловинний атом кремнію (C+I) поблизу фронту кристалізації для бездислокаційних монокристалів кремнію, що отримані методами безтигельної зонної плавки та Чохральського. Наведені аналітичні вирази узгоджуються з гетерогенним механізмом утворення ростових мікродефектів.