

On the Problem of the Consistency of the High-Temperature Precipitation Model with the Classical Nucleation Theory

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Abstract—The adequacy of the model of high-temperature precipitation in dislocation-free silicon single crystals to the classical theory of nucleation and growth of second-phase particles in solids has been considered. It has been shown that the introduction and consideration of thermal conditions of crystal growth in the initial equations of the classical nucleation theory make it possible to explain the precipitation processes occurring in the high-temperature range and thus extend the theoretical basis of the application of the classical nucleation theory. According to the model of high-temperature precipitation, the smallest critical radius of oxygen and carbon precipitates is observed in the vicinity of the crystallization front. Cooling of the crystal is accompanied by the growth and coalescence of precipitates. During heat treatments, the nucleation of precipitates starts at low temperatures, whereas the growth and coalescence of precipitates occur with an increase in the temperature. It has been assumed that the high-temperature precipitation of impurities can determine the overall kinetics of defect formation in other dislocation-free single crystals of semiconductors and metals.

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1. INTRODUCTION

The presence of structural imperfections in dislocation-free silicon single crystals significantly affects their mechanical, electrical, optical, and other properties. As is known, cooling of dislocation-free silicon single crystals during their growth is accompanied by the formation of grown-in microdefects. The formation of grown-in microdefects is caused by complex processes of interactions between intrinsic point defects (vacancies and interstitial silicon atoms) and impurity atoms of oxygen and carbon in cooling silicon ingots. Depending on the thermal conditions of crystal growth, grown-in microdefects are precipitates of impurities, microvoids, or interstitial dislocation loops [1].

The problem of the formation of grown-in microdefects has both the technological aspect (control of the defect structure of the crystal during the growth for the purpose to increase its quality) and the fundamental scientific importance, because its solution makes it possible to describe the physics of defect formation in ultra-pure dislocation-free silicon single crystals. The construction of a theoretical model of the formation of grown-in microdefects in dislocation-free silicon single crystals is an important scientific and practical problem from the viewpoint of the development of physical principles of the purposeful creation of new materials with a desired set of physical properties.

Currently, there are two theoretical models of the formation of grown-in microdefects, which are based on two physical approaches: the recombination–dif-

fusion model [2] and the two-stage (heterogeneous) mechanism [3]. The recombination–diffusion model is based on the priority of intrinsic point defects in the formation of grown-in microdefects. The rapid recombination of intrinsic point defects in the vicinity of the crystallization front leads to the formation of microvoids or dislocation loops, depending on the thermal conditions of the crystal growth (the growth parameter V/G , where V is the growth rate of the crystal and G is the axial temperature gradient at the crystallization front) [2, 4]. During cooling of the crystal, no precipitation of impurities occurs [5, 6]. The subsequent heat treatments of silicon mainly result in the formation of oxygen precipitates (SiO_2). The recombination–diffusion model was used to construct different modifications of the mathematical model of the dynamics of point defects [7].

The two-stage mechanism of the formation of grown-in microdefects denies recombination of intrinsic point defects in the vicinity of the crystallization front [3, 8]. As a result, the decomposition of supersaturated solid solutions of point defects proceeds in two directions associated with the precipitation of oxygen and carbon (SiC) [9]. The formation of microvoids or dislocation loops is possible at lower cooling temperatures, depending on the thermal conditions of crystal growth [10]. The mathematical models of the formation of precipitates, microvoids, and dislocation loops, in combination with the two-stage mechanism, represent the diffusion model of the formation of grown-in microdefects [11]. The diffusion

model is based on the model of high-temperature precipitation [8]. However, the question arises about the adequacy of this model to the general theoretical concepts of nucleation processes.

The purpose of this work was to demonstrate that the high-temperature precipitation of impurities is consistent with the classical theory of nucleation and growth of second-phase particles and, in turn, extends the field of its application to the processes of cooling of the solid.

2. RECOMBINATION–DIFFUSION MODEL AND NUCLEATION THEORY

The decomposition of the solid solution begins with the nucleation, i.e., the formation of physically distinguishable centers, which then grow. This growth leads to the precipitation of a new phase within the initial solid solution. The precipitation of the second phase occurs in three stages: (i) the local fluctuation of the chemical potential (the formation of a nucleus), (ii) the formation of a stable nucleus, and (iii) the growth and coalescence of precipitates [12].

The change in the free energy of the crystal ΔG due to the formation of a nucleus has the form

$$\Delta G = \Delta G_V + \Delta G_S + \Delta G_L, \quad (1)$$

where ΔG_V is the change in the free energy due to the variation of the chemical composition in the volume (the quantity has a negative sign), ΔG_S is the change in the free energy due to the formation of an interface, and ΔG_L is the change in the free energy due to the variation in the volume of the nucleus [12]. After substituting the expressions derived for the quantities ΔG_V , ΔG_S , and ΔG_L into formula (1), we obtain

$$\Delta G = \alpha R^3 (\Delta g_V + \Delta g_L) + \beta R^2 \Delta g_S, \quad (2)$$

where α is the geometric factor that takes into account the shape of the nucleus, β is the shape factor of the nucleus, R is the linear characteristic size of the nucleus, Δg_V is the difference between the volume energies of the phases per unit volume, Δg_S is the surface energy of the nucleus per square centimeter, and Δg_L is the difference in the elastic energies of the nucleus and the crystal per unit volume. When the inequality $|\Delta g_L| > |\Delta g_V|$ is satisfied, the formation of the nucleus begins to occur. In this case, the dependence $\Delta G(R)$ has the shape of a curve with the maximum corresponding to the critical nucleus size R_c . If the nucleus size satisfies the inequality $R < R_c$, the nuclei will dissolve. If the nucleus size satisfies the inequality $R > R_c$, the nuclei will grow [12].

The critical nucleus size R_c can be found from the condition of the maximum of the curve $d\Delta G(R)/dR = 0$:

$$R_c = \left| \frac{2\beta\Delta g_S}{3\alpha(\Delta g_V + \Delta g_L)} \right|. \quad (3)$$

Then, the corresponding energy is given by the expression $\Delta G_c = 3\beta R_c^2 \Delta g_S$. It can be shown that $\Delta G_V = kT \ln(C_X/C_X^{\text{eq}})$, where C_X is the impurity concentration; C_X^{eq} is the equilibrium impurity concentration, which depends on the temperature; k is the Boltzmann constant, and T is the temperature [6, 12]. Hence, we can write

$$R_c = \frac{2\beta\Delta g_S}{kT \ln(C_X/C_X^{\text{eq}})}. \quad (4)$$

A more complete theoretical treatment of the critical size of a nucleus is given in [13]:

$$R_c = \frac{2\sigma u V_p}{kT \ln(S_X S_i^{-\gamma_i} S_v^{-\gamma_v}) - 6\mu\delta\epsilon u V_p}, \quad (5)$$

where $S_X = C_X/C_X^{\text{eq}}$, $S_i = C_i/C_i^{\text{eq}}$, and $S_v = C_v/C_v^{\text{eq}}$ are the supersaturations of impurity atoms, self-interstitial silicon atoms, and vacancies, respectively; σ is the surface energy density of the interface between the precipitate and the matrix; μ is the shear modulus of silicon; δ and ϵ are the relative linear and volumetric misfit strains of the precipitate and the matrix, respectively; γ_i and γ_v is the fractions of self-interstitial silicon atoms and vacancies per impurity atom attached to the precipitate, respectively; V_p is the molecular volume of the precipitate; and $u = (1 + \gamma_i x + \gamma_v x)^{-1} \left(\frac{1 + \epsilon}{1 + \delta} \right)^3$.

From expressions (4) and (5), it follows that the critical nucleus size increases with an increase in the temperature [6]. However, at low cooling temperatures, where the diffusion is slow, the nucleation rate is negligible [6]. In the medium-temperature range $T \sim 1400$ – 1000 K, the homogeneous formation of microvoids or dislocation loops occurs [5]. In the framework of the recombination–diffusion model, it is assumed that cooling of the silicon single crystal in the high-temperature range $T \sim 1682$ – 1400 K can lead to the formation of very small nuclei of microvoids or dislocation loops [2, 4, 7]. In [14, 15], an attempt was made to justify theoretically the formation of complexes “vacancy + oxygen” and “vacancy + nitrogen” at temperatures below the temperatures of formation and growth of microvoids or dislocation loops. It is assumed that subsequent heat treatments result in the transformation of these complexes into precipitates.

On the other hand, there is a large amount of experimental data obtained in our earlier studies [1, 16] and in a number of studies by other authors [17–21]. These experimental studies of grown-in microdefects demonstrated that the precipitation of impurities occurs immediately during cooling of the crystal after the growth. It is well known that silicon is a high-purity material whose properties and structure are deter-

mined by the concentration of impurities. In the high-temperature range, the concentrations of oxygen and carbon impurities in the crystals grown by the Czochralski method are several orders of magnitude higher than the concentrations of intrinsic point defects.

3. HIGH-TEMPERATURE PRECIPITATION AND THE NUCLEATION THEORY

The absence of recombination of intrinsic point defects in the high-temperature range leads to the fact that, during the cooling of the crystal after passing through the diffusion zone, an excessive (nonequilibrium) concentration of intrinsic point defects appears. Excess intrinsic point defects disappear at sinks whose role in this process is played by uncontrollable (background) impurities of oxygen and carbon [1, 3]. The calculations performed in the framework of the model of dissociative diffusion–migration of impurities showed that the edge of the reaction front of the formation of a complex (oxygen–vacancy and carbon–interstitial silicon atom) is located at a distance of $\sim 3 \times 10^{-4}$ mm from the crystallization front [22]. The results of calculations of the Fokker–Planck partial differential equations confirm that the processes of nucleation occur very rapidly in the vicinity of the crystallization front [8].

The minimum size of the critical nucleus is observed in the initial state at $T = 1682$ K and increases with a decrease in the temperature [8]. In our previous paper [9], we considered the problems associated with the growth of nuclei and the coalescence of precipitates. The performed analysis of the calculated curves demonstrated that there is good agreement between the experimental and calculated data. This relates to the temperatures of formation of primary grown-in microdefects, experiments on quenching of crystals, the concentrations of $(I + V)$ -microdefects and $D(C)$ -microdefects determined from the results of electron microscopy investigations ($\sim 10^{13}$ cm $^{-3}$), and the final sizes of all types of microdefects [1].

We showed that the precipitation process (the nucleation, growth, and coalescence of particles of a second phase) occurs over the entire temperature range of cooling of the crystal ($T \sim 1682$ – 300 K) after the growth [23]. This process can be slowed down or suspended in a narrow temperature range (at temperatures $T \leq T_m - 300$ K, where T_m is the crystallization temperature) where, depending on the thermal parameters of the crystal growth, there arise conditions for the homogeneous formation of microvoids or dislocation loops [4, 5]. In this case, the presence of the already formed precipitates in the crystal at temperatures $T \leq T_m - 300$ K leads to the fact that the formation of dislocation loops predominantly occurs according to the deformation mechanism [24]. Consequently, the process of high-temperature precipita-

tion of impurities determines the defect structure of the crystal during the growth and subsequent technological processing.

However, from the publications on the simulation of precipitation of impurities at high cooling temperatures [8, 11], it is not clear what physical principles underlie the consistency with the classical theory of nucleation and whether this consistency exists altogether.

4. EXPERIMENTAL RESULTS AND DISCUSSION

In the calculations, we used the following data: $V_p = 4.302 \times 10^{-2}$ (SiO $_2$) and 2.04×10^{-2} nm 3 (SiC), $\sigma = 310$ (SiO $_2$) and 1000 erg/cm 2 (SiC), $\mu = 6.41 \times 10^{10}$ Pa, $\delta = 0.3$, $\varepsilon = 0.15$, $b = 0.25$ nm, $C_O^{eq} = 9 \times 10^{22} \exp(-1.52/kT)$, $D_O = 0.17 \exp(-2.54 \text{ eV}/kT)$, $D_C = 1.9 \exp(-3.1 \text{ eV}/kT)$, and $k = 8.6153 \times 10^{-5}$ eV/K, where D_O and D_C are the diffusion coefficients of oxygen and carbon, respectively; C_O^{eq} is the equilibrium concentration of the oxygen impurity; and k is the Boltzmann constant.

The analysis was carried out in the following approximation: the growth of precipitates occurs on a fixed number of nucleation centers according to the diffusion growth mechanism. The model was designed for the uniform precipitation throughout the volume. We performed two groups of calculations, which simulated the processes of precipitation during the growth of crystals with large and small diameters using the Czochralski method (CZ-Si) and the floating zone method (FZ-Si). In the calculations of the first group, we used the following parameters: the crystal growth rate was $V = 0.6$ mm/min, the axial temperature gradient was $G = 2.5$ K/mm, and the concentrations of oxygen and carbon were $C_O = C_C = 10^{18}$ cm $^{-3}$ (hereinafter, crystals of group I). In the calculations of the second group, we used the crystal growth rate $V = 6$ mm/min, the axial temperature gradient $G = 130$ K/cm, the oxygen concentration $C_O = 8 \times 10^{16}$ cm $^{-3}$, and the carbon concentration $C_C = 10^{16}$ cm $^{-3}$ (hereinafter, crystals of group II).

As is known, the formation and development of the structure of grown-in microdefects in silicon are determined by thermal conditions of growth and cooling of the crystal. This was proved experimentally and has been questioned neither in the model of the dynamics of point defects [4, 5] nor in the diffusion model [11]. The temperature distribution along the length of the ingot during its cooling varies depending on the thermal parameters of the growth according to the expression $1/T = 1/T_m + GZ/T_m^2$, where Z is the distance from the crystallization front [2]. It should be noted that, in the general case, it is necessary to take

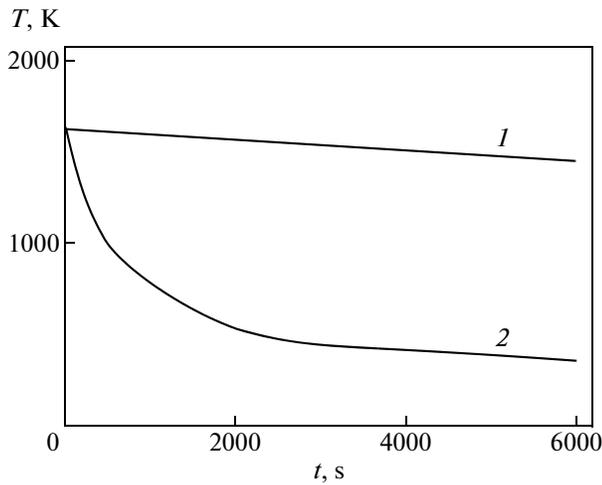


Fig. 1. Axial temperature distributions in crystals of groups (1) I and (2) II.

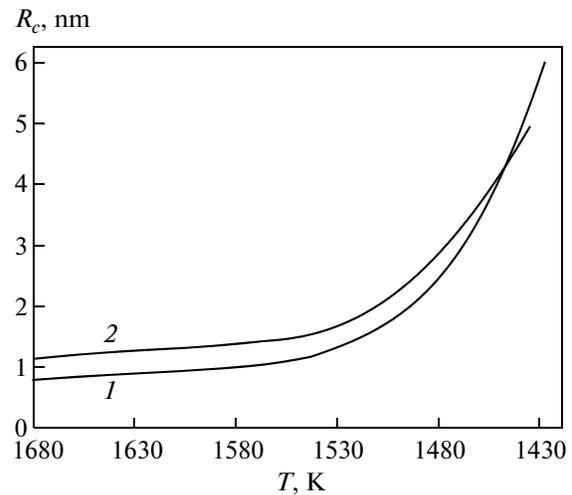


Fig. 2. Temperature dependences of the critical radii of (1) oxygen precipitates and (2) carbon precipitates for the crystal of group I.

into account the radial inhomogeneity of the temperature field. We introduce the crystal growth rate into in this formula and obtain

$$T(t) = \frac{T_m^2}{T_m + VGt}. \quad (6)$$

In this case, the growth parameter V/G is the parameter controlling the process of defect formation in silicon. At the same time, in the framework of the recombination–diffusion model, this parameter is interpreted only as a criterion that separates the regions of the existence of microvoids and dislocation loops. The dependences $T(t)$ for the crystals of groups I and II are shown in Fig. 1.

The observed difference in the dependences $T(t)$ leads to the formation of different defect structures in the crystals of groups I and II. For example, in the crystal of group I (diameter 200 mm), microvoids are formed in the central part, whereas dislocation loops are formed in regions near the surface. At the same time, oxygen and carbon precipitates are formed both in the center and on the edges of the crystal. However, the crystal of group II contains only the carbon and oxygen precipitates [1, 3].

We introduce the dependence $T(t)$ into expression (5) taking into account that the concentrations C_v^{eq} and C_i^{eq} depend on the temperature T , that is,

$$R_c = \frac{2\sigma u V_p}{kT(t) \ln(S_X S_i^{-\gamma_i} S_v^{\gamma_v}) - 6\mu\delta\epsilon u V_p}. \quad (7)$$

Figure 2 shows the calculated temperature dependences of the critical radii of the oxygen and carbon precipitates in the crystal of group I.

The minimum values of the critical radii $R_c = 0.81$ nm (oxygen precipitate) and $R_c = 1.1$ nm (carbon precipitate) are reached in the initial state at $T = 1682$ K and increase with a decrease in the temperature. At $T \approx 1455$ K, the critical radii of the oxygen and carbon precipitates become equal to each other (~ 3.6 nm), and then, as the temperature decreases, the critical radius of oxygen precipitates increases more rapidly. An increase in the critical radius of the precipitates during the cooling of the crystal leads to a sharp decrease in the rate of their growth and, consequently, to a drastic decrease in the precipitation rate. Previously, it was shown that the stage of the coalescence of large-sized silicon single crystals begins to occur at temperatures close to the temperatures of the formation of clusters of intrinsic point defects [9].

For the crystal of group II, the slightly higher minimum values of the critical radii $R_c = 0.813$ nm (oxygen precipitate) and $R_c = 1.107$ nm (carbon precipi-

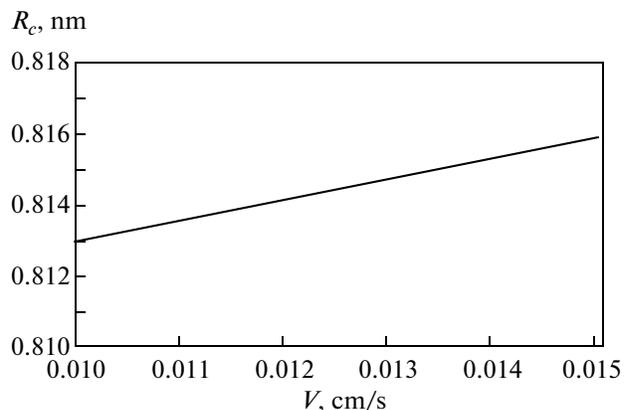


Fig. 3. Dependence of the critical radius of oxygen precipitates in the crystal of group II ($G = \text{const}$ and $T = 1682$ K) on the growth rate.

tate) are reached in the initial state at $T = 1682$ K and also increase with a decrease in the temperature. For both groups of crystals, the minimum values of R_c (at $T = 1682$ K) increase with increasing growth rate of the crystal or axial temperature gradient at the crystallization front. As an example, Fig. 3 shows the dependence $R_c(V)$ for oxygen precipitates at constant values of the axial temperature gradient G and temperature $T = 1682$ K. It should be noted that the higher is the value of V (or G), the more rapid is the increase in the value of the function $R_c(V)$ or $R_c(G)$ in crystals of both groups.

It is well known that the first-order phase transition occurs through the stage of the formation of the so-called activated complex [25]. This state corresponds to the highest saddle point of the lowest energy barrier separating the initial (reagents) and new (reaction products) phases in the reaction coordinate space. For the conventional first-order phase transition, the activated complexes are critical nuclei of the new phase in the volume of the initial phase; i.e., activated complex is inhomogeneous or heterogeneous [26].

If the first-order phase transition occurs in a solid, then, for the formation of a nucleus of the new phase, it is necessary to take into account the elastic stresses generated in both the nucleus and the matrix of the initial material. Moreover, if the elastic energy or other factors drastically increase the energy of formation of critical nuclei directly in the initial phase, this inhomogeneous state ceases to play the role of an activated complex for the chemical reaction or phase transition, because these nuclei cease to correspond to the lowest energy barrier separating the initial and new phases [26].

This situation becomes possible in the case when the crystal structure of the new phase differs from the crystal structure of the initial phase and when the density of the new phase is less than the density of the initial phase, as well as in the case of the incoherent matching between the crystal lattices of the new and old phases. This point relates to the use of formula (5), because it holds true only for the case of coherent phase matching.

Under these conditions, a homogeneous state is formed from the initial state and plays the role of an intermediate state; then, from this state, nuclei of the final phase are formed, i.e., a new activated complex [27].

In particular, it was shown in [27] that the transition from silicon to silicon carbide occurs through an intermediate state, which includes silicon saturated with dilatation dipoles, i.e., stable objects consisting of a carbon atom, which is located in a silicon interstitial, and a silicon vacancy. Owing to the elastic dilatation energy and the elastic energy due to the coherent matching, the energy of formation of the SiC critical nucleus directly in silicon is very high. The saturation of silicon with dilatation dipoles smoothly decreases the barrier for the formation of SiC down to the values close to kT , after which the formation of SiC from a

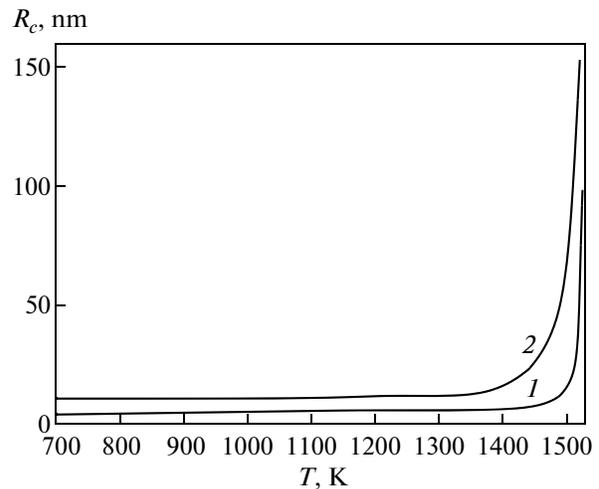


Fig. 4. Dependences of the critical radii of (1) oxygen precipitates and (2) carbon precipitates on the heat treatment temperature.

homogeneous intermediate state occurs very rapidly over the entire volume of the intermediate state [27]. It should be taken into account that, in the high-temperature range, this barrier is significantly lower than the barrier for the recombination of intrinsic point defects [28].

Previously, we proposed a kinetic model of the formation and growth of interstitial dislocation loops, according to which the formation and development of dislocation loops are caused by the high-temperature precipitation of background impurities when there is a mismatch between the lattice parameters of the crystal matrix and the precipitate [24]. The accumulation of the elastic energy during the growth of the precipitate results in a loss of coherence with the matrix, when it is impossible to establish a one-to-one correspondence between the atoms on different sides of the interface. This leads to a structural relaxation of precipitates through the formation and motion of dislocation loops. The growth and coalescence of dislocation loops occurs primarily due to the generation of interstitial silicon atoms by growing precipitates, as well as due to the dissolution of small dislocation loops [24].

It can be seen that the model of high-temperature precipitation does not contradict the classical nucleation theory and even extends the scope of its applicability to the nucleation of second-phase particles during cooling of the crystals. Therefore, the diffusion model of the formation of grown-in microdefects, which is constructed based on the model of high-temperature precipitation, should be general and universal in character. This means that the diffusion model should consider the formation and development of a defect structure during the growth of the crystal and its technological processing within a unified context. In our recent paper [29], we considered the mathematical formalism of the diffusion model of the formation

of grown-in microdefects as applied to the formation of a defect structure of an undoped dislocation-free silicon single crystal upon heat treatments.

In the calculation equations, we introduce values $T = \text{const}$ instead of dependence (6). Then, in particular, when determining the critical radius of precipitates, we return to expression (5). Figure 4 shows the dependences of the critical radii of the oxygen and carbon precipitates on the heat treatment temperature [29].

During the heat treatment at a temperature $T = 730$ K, the size of the critical nucleus of an oxygen precipitate is equal to 2.7 nm, whereas the size of the critical nucleus of a carbon precipitate is approximately 8.7 nm. The minimum values of the critical radii of the precipitates are reached in the initial state at $T = 730$ K and increase with increasing temperature. An increase in the annealing temperature of the crystals leads to an increase in the size of critical nuclei of the precipitates. Furthermore, with an increase in the oxygen concentration at a constant annealing temperature, the size of critical nuclei decreases [29].

The kinetics of precipitation during the heating of the crystal is similar to the kinetics of precipitation during the cooling of the crystal in the process of its growth. However, the results of calculations, together with the large value of the critical nucleus size of the carbon precipitates as compared to the critical nucleus size of the oxygen precipitates, can indicate that, during heat treatments, predominantly the oxygen precipitation occurs [29].

In [29], we considered a hypothetically defect-free crystal. Real silicon single crystals contain grown-in microdefects that, during heat treatments, serve as sinks for intrinsic point defects and impurity atoms. Therefore, the growth of precipitates formed during the growth of the single crystal can occur simultaneously with the formation of new precipitates. The transformation and formation of precipitates during heat treatment leads to supersaturation of the crystal with self-interstitial atoms. This process, depending on the conditions of formation of the initial defect structure and parameters of the heat treatment, causes the formation and growth of dislocation loops and stacking faults, as well as a decrease in the size or dissolution of microvoids [11, 21].

Therefore, the high-temperature precipitation of oxygen and carbon is a fundamental process in the formation of a defect structure of silicon during cooling of the crystal after the growth. The model of high-temperature precipitation, together with the deformation model of the formation of dislocation loops and the homogeneous model of the formation of microvoids, is adequate to the experimental results of the investigation of the defect structure of silicon single crystals [11].

The inclusion of thermal growth conditions of silicon single crystals in the form of the dependence $T(t)$ allows us to theoretically describe the conditions for nucleation, growth, and coalescence of the precipi-

tates in the range from the crystallization temperature to room temperature. In this case, the Vanhellemont–Claeys model [13] is not only applicable to the description of the nucleation of precipitate nuclei in silicon during heat treatments but also is extended to the processes of cooling of the crystal during the growth. According to this model, the interaction of point defects with each other occurs already at the initial stage of cooling of the crystal. The interaction of impurities with intrinsic point defects has a fundamental character and determines the defect structure of the crystal from the onset of the crystallization to the fabrication of the finished device.

A comprehensive theoretical description of the defect formation is provided by the diffusion model, which is based on the model of high-temperature precipitation. From our analysis, it follows that the model of high-temperature precipitation is not only adequate to the experimental results of the investigation of grown-in microdefects but also does not contradict the classical theory of nucleation of second-phase particles. Furthermore, this model extends the field of application of the mathematical apparatus of the classical nucleation theory to the formation of nuclei in a solid during its cooling after the growth.

The correction of traditional concepts about the dominant role of intrinsic point defects showed that semiconductor silicon—a highly pure material with the perfect structure—can be considered as the initial model for the construction of theoretical models of defect formation in other semiconductor materials and metals. The obtained mathematical models and methods proposed for their solution in silicon make it possible to formulate and solve many problems on the kinetics of diffusion processes in solids. We believe that the diffusion model has a general character and is applicable to the mathematical description of processes such as precipitation of impurities, void formation, formation of dislocation loops in crystals, and others. The diffusion model provides an adequate description of the interaction between intrinsic point defects and impurities, as well as the modification of a defect–impurity system during cooling of the crystal after the growth. The primacy of the processes of high-temperature precipitation is a fundamental feature that determines the overall kinetics of defect formation in highly perfect crystals of semiconductors and metals. The generality of the approach does not exclude specific features of the application of the diffusion model for different materials, which are associated with different thermal growth conditions and different types of crystal structures. The specificity of growth and the difference in the crystal structures of different dislocation-free single crystals must necessarily be taken into account in the physical model and mathematical constructions of the diffusion model.

A brief analysis of two theoretical models of defect formation in silicon and the results obtained in this

study allow us to conclude that the model of the dynamics of point defects is a special case of the diffusion model for the explanation of the homogeneous formation of microvoids.

5. CONCLUSIONS

The model of high-temperature precipitation and the classical nucleation theory mutually complement and extend the capabilities of theoretical description of the nucleation in solids. The introduction and consideration of thermal conditions of crystal growth in the initial equations of the classical nucleation theory make it possible to demonstrate that the formation of critical nuclei of small sizes, with a higher probability, occurs in the vicinity of the crystallization front. Cooling of the crystal is accompanied by the growth and coalescence of precipitates. The initial defect crystal structure is formed depending on thermal growth conditions and, in the general case, includes grown-in defects, such as precipitates of impurities, dislocation loops, and microvoids.

During heat treatments of single crystals, the formation of critical nuclei of small sizes occurs at low temperatures. In this case, an increase in the temperature leads to the growth and coalescence of precipitates. The real defect structure of the crystal is determined by the transformation of initial grown-in defects and by the formation of new imperfections after different heat treatments.

At present, from the viewpoint of the classical theory of nucleation of second-phase particles in solids, the diffusion model of defect formation provides a comprehensive theoretical description of the nucleation and development of a defect structure both at the stage of growth of the crystal and at the stage of its technological processing. This opens up unique opportunities for monitoring and controlling the process of defect formation in crystals beginning with the growth stage and ending with the fabrication of the device.

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