

High-Temperature Precipitation of Impurities in Metals

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Abstract—Using two alternative approaches to describing the defect structure of dislocation-free copper single crystals (the classical theory of the nucleation and growth of particles of the second phase in solids and Vlasov’s model for solids), we demonstrated that high-temperature precipitation of impurities occurs upon cooling of a growing crystal. High-temperature precipitation of impurities can lead to further development of a defective crystal structure due to the formation of dislocation loops, microvoids (or micropores), dislocations, etc.

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INTRODUCTION

Recently, we have created a diffusion model of defect formation in dislocation-free silicon and germanium single crystals [1–3]. This model can be used to describe the behavior of structural imperfections during both crystal growth and the creation of device structures.

The diffusion model of defect formation is based on the model of high-temperature precipitation of impurities. Precipitates formed near the crystallization front are responsible for the formation of a defective crystal structure. Upon crystal cooling, precipitates transform and, depending on various thermal conditions of growth, can form micropores and dislocation loops [1]. Thermal and radiation treatments of crystals during the creation of device structures cause the transformation of dislocation loops into dislocations, stacking defects, etc. [4]. The theoretical consideration of the diffusion model was based on two theories of defect formation in solids. These two theories (classical [5, 6] and probabilistic [7]) were based on completely different physical principles. However, they led to identical results and confirmed the fact that high-temperature precipitation is primary in the creation of a defect structure in silicon and germanium crystals [3, 8]. We assumed that high-temperature precipitation forms the site of defect formation in crystals of various types. This assumption primarily concerns high-temperature precipitation in metal crystals. The issues of precipitation of impurities in metals and metal alloys are being actively studied (see, for example, [9–11]). Sajadi et al. [12] considered the alloying of the Cu–Ni–Si alloy with chromium, iron, aluminum, and manganese, followed by a computational

experiment. The authors calculated cases of pairwise mixing of all elements to study the effect of impurities on the electrical conductivity and strength of the matrix. The saturation of the copper melt with oxygen and the synthesis of chromium carbide to study the effect of chromium carbide and oxygen on the mechanical properties of the matrix were discussed in [13]. These works are undoubtedly essential in light of the goals pursued by the authors. However, knowledge of the initial defect structure of the matrix formed at the initial moment of crystallization of the grown crystal is of no less importance. Any subsequent impact on the crystals, in particular, doping, leads to the formation of additional precipitates, that is, structural imperfections. When studying the effect of additional processing on the properties of the matrix, we should take into account its interaction with the already existing defect structure. The main problem of the theory of precipitation, as such, is the insufficient attention of some authors to the primary (initial) defective structure of the base material and the study of only the secondary defective structure introduced through additional processing. As applied to semiconductor materials, before our series of works, several authors completely denied the fact of high-temperature precipitation. Nevertheless, in crystals with a covalent bond, the initial defective structure was precisely high-temperature precipitates formed at the initial time of crystallization after crystal growth, that is, in the absence of any additional external effects. Thus, the purpose of this work is to prove the possibility of high-temperature precipitation in metals using the classical and probabilistic approaches by demonstrating the possibility of creating stable impurity complexes at high temperatures. This problem is relevant from the point of view of the need to consider the initial defect

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structure of the matrix during its interaction with the secondary defect structure and for establishing the identity of defect formation in crystals with covalent and metallic bonds.

CLASSICAL APPROACH

In the classical approach, the concept of a crystal lattice is introduced. It is assumed that the atoms are located at the nodes of the crystal lattice, and their totality is an integer. The mechanical description of the behavior of particles and the concept of probability do not contradict each other [5]. Born's theory of crystals led, in particular, to the creation of the classical theory of the nucleation and growth of particles of the second phase in solids [6]. The diffusion model created based on this classical theory describes the formation and development (transformation) of a defective structure of a solid both during its growth and by various technological effects [1].

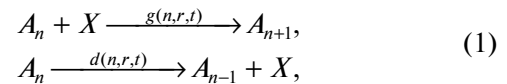
The crystal structure of metals in comparison with semiconductors has particular characteristics. If semiconductors (for example, silicon or germanium) have a loose crystalline structure, metals are distinguished by a denser packing of atoms. Consequently, both types of intrinsic point defects (vacancies and self-interstitials) can coexist in semiconductors at comparable concentrations. However, since the energy of formation of vacancies in the closest packings of metals is several times less than the energy of formation of self-interstitials, the formation of the latter is hindered, and vacancies become the main point defects.

When crystals grow from a melt, dislocations form. The concentration and distribution of dislocations are determined by the thermal conditions of crystal growth. They can form by various mechanisms. However, plastic deformation caused by thermal stress is the main mechanism of crystal growth. Regardless of the source of stress σ , their occurrence causes elastic deformation $\varepsilon = \sigma/E$, where E is the modulus of elasticity. If this stress exceeds a certain value of the yield strength, plastic deformation occurs accompanied by the formation of dislocations. Near the melting point, the yield strength of metals is close to zero, which contributes to a much easier formation of dislocations compared to covalent crystals, causing great difficulties in growing dislocation-free metal single crystals.

The use of a narrow waist and a system of shielding devices in Czochralski method significantly lowers the axial and radial temperature gradients, and thermal stress could be decreased to a level insufficient for the formation of dislocations [14]. Based on this data, large (6–8 mm in diameter and 60 mm in length) dislocation-free single crystals of copper were obtained. Previously, similar results [15–17] enabled a conclusion about the heterogeneous mechanism of dislocation formation.

Let us consider a hypothetical dislocation-free single crystal of copper. The concentrations of all point defects at the crystallization front are in equilibrium. Differences in the concentrations of vacancies and self-interstitials near the crystallization front make it possible to consider only one (vacancy) branch of defect formation in calculations, in contrast to covalent crystals. When the crystal is cooled after passing through the diffusion zone, an excess (nonequilibrium) concentration of vacancies arises. The disappearance of excess vacancies occurs on the drains, the role of which is played by various impurities. The formation of complexes between intrinsic point defects and impurities is determined, on the one hand, by the fact that both are sources of internal stress in the lattice (elastic interaction), and, on the other hand, by Coulomb interaction between them (if defects and impurities are present in a charged state). We take into account only the elastic interaction and the oxygen impurity, which is always present in crystals.

Let us consider an approach based on systems of interrelated discrete differential equations of quasi-chemical reactions for describing the initial stages of the formation of nuclei of new phases and a similar system of continual differential equations of Fokker–Planck type. The formation of precipitates can be represented as a reaction that consists of random processes of attachment and detachment of particles X ,



where A_n is cluster A consisting of n particles X ; $g(n, r, t)$ is the growth rate of cluster A_n ; $d(n, r, t)$ is the decay rate of cluster A_n . The concentration of clusters A_n at a point r is determined by the function $f(n, r, t)$. Then the change of this function in time is a system of differential equations

$$\frac{\partial f(n, r, t)}{\partial t} = J(n, r, t) - J(n+1, r, t) \quad (n = 2, 3, \dots, n_{\max}), \quad (2)$$

$$J(n, r, t) = g(n-1, r, t)f(n-1, r, t) - d(n, r, t)f(n, r, t).$$

Conservation of the number of particles is

$$\frac{\partial f(1, r, t)}{\partial t} = -J(2, r, t) - \sum_{n=2}^{n_{\max}} J(n, r, t), \quad (3)$$

where n_{\max} is the maximum number of particles X contained in cluster A .

The system of discrete equations can be represented by a continuum partial differential equation (Fokker–Planck equation) [18],

$$\frac{\partial f(n, r, t)}{\partial t} = -\frac{\partial I(n, r, t)}{\partial n}. \quad (4)$$

Here,

$$I(n, r, t) = Af - B \frac{\partial f}{\partial n}, \quad (5)$$

$$A = g - d - \frac{\partial B}{\partial n}, \quad B = \frac{g + d}{2}. \quad (6)$$

The linking of Eqs. (2) and (4) occurs at $n = n_{\min}$; then the particle conservation law (3) is

$$\begin{aligned} \frac{\partial f(1, r, t)}{\partial t} &= -J(2, r, t) \\ &- \sum_{n=2}^{n_{\min}-1} J(n, r, t) - \int_{n_{\min}}^{n_{\max}} I(n, r, t) dn. \end{aligned} \quad (7)$$

The system of equations (2)–(7) makes it possible to consider the processes of nucleation and subsequent growth of clusters within the framework of a single model. To simplify the calculations, we consider the case of a thin plane-parallel crystal plate of a large diameter, when the conditions in the plane parallel to the crystal surface can be considered homogeneous, and diffusion can be considered only along the normal to the surface (coordinate axis z). The mass balance of point defects in the crystal is described by a system of diffusion equations for oxygen atoms and vacancies

$$\begin{aligned} \frac{\partial C_O}{\partial t} &= D_O \frac{\partial^2 C_O}{\partial z^2} - \frac{\partial^2 C_O^{\text{Cu}_2\text{O}}}{\partial t}, \\ \frac{\partial C_v}{\partial t} &= D_v \frac{\partial^2 C_v}{\partial z^2} - \frac{\partial^2 C_v^{\text{Cu}_2\text{O}}}{\partial t}, \end{aligned} \quad (8)$$

where C_v , C_O are the concentrations of vacancies and oxygen in the crystal, respectively; D_v , D_O are the diffusion coefficients of vacancies and oxygen, respectively; $C_v^{\text{Cu}_2\text{O}}$, $C_O^{\text{Cu}_2\text{O}}$ are the concentrations of vacancies and oxygen in precipitates.

The system of interrelated Fokker–Planck equations can be converted to a dimensionless form

$$\frac{\partial \tilde{f}_{\text{Cu}_2\text{O}}}{\partial \tau} = -\frac{\partial I_{\text{Cu}_2\text{O}}}{\partial \tilde{v}_O}. \quad (9)$$

The normalized sizes of precipitates are defined in Eq. (9) as $\tilde{v}_O = n_O/n_O^{\text{cr},0}$, where n_O^{cr} is the normalized critical size of precipitates. The critical rate of growth of precipitates, $g_{\text{Cu}_2\text{O}}^0 = N_O^0 v_O \exp(-G_{\text{act}}^{\text{Cu}_2\text{O}}/kT)$, where $N_O^0 = 4\pi(r_O^{\text{cr},0})^2 \delta_{\text{Cu}_2\text{O}} C_O^{\text{eq}}$ is the number of particles near the precipitate with critical sizes.

The size distribution function of precipitates in Eq. (9) is normalized to the initial concentrations of nucleation centers $\tilde{f}_{\text{Cu}_2\text{O}} = f_{\text{Cu}_2\text{O}}/f_{\text{Cu}_2\text{O}}^0$. The particle fluxes on the right side of Eq. (9) are $A_{\text{Cu}_2\text{O}} = (\tilde{g}_{\text{Cu}_2\text{O}} - \tilde{d}_{\text{Cu}_2\text{O}})n_O^{\text{cr},0} - \partial B_{\text{Cu}_2\text{O}}/\partial \tilde{v}_O$, where the following notations are used for the normalized kinetic coefficients:

$$\begin{aligned} A_{\text{Cu}_2\text{O}} &= (\tilde{g}_{\text{Cu}_2\text{O}} - \tilde{d}_{\text{Cu}_2\text{O}})n_O^{\text{cr},0} - \partial B_{\text{Cu}_2\text{O}}/\partial \tilde{v}_O; \quad B_{\text{Cu}_2\text{O}} = \\ &(\tilde{g}_{\text{Cu}_2\text{O}} + \tilde{d}_{\text{Cu}_2\text{O}})/2; \quad \tilde{g}_{\text{Cu}_2\text{O}} = g_{\text{Cu}_2\text{O}}/g_{\text{Cu}_2\text{O}}^0; \quad \tilde{d}_{\text{Cu}_2\text{O}} = \\ &d_{\text{Cu}_2\text{O}}/g_{\text{Cu}_2\text{O}}^0. \end{aligned}$$

The critical size of precipitates can be determined by the equation [19]

$$r_O^{\text{cr}} = \frac{2\sigma u V_p}{kT \ln(S_O S_v^{\gamma_v}) - 6\mu\delta\epsilon u V_p}, \quad (10)$$

where $S_O = C_O/C_O^{\text{eq}}$; $S_v = C_v/C_v^{\text{eq}}$ are supersaturations of oxygen atoms and vacancies, respectively; σ is the surface energy density of the interface between the precipitate and the matrix; μ is a copper shear module; δ and ϵ are linear and volumetric deformations of the precipitate and matrix mismatch; γ_v is the fraction of vacancies per one impurity atom attached to the precipitate; V_p is the volume of the precipitate molecule;

$u = (1 + \gamma_v x + \gamma_v x)^{-1} \left(\frac{1 + \epsilon}{1 + \delta} \right)^3$. The number of impurity atoms in compressed precipitates with radii r_O is defined as

$$n_O = \frac{4\pi r_O^3 (1 + \gamma_v x) \left(\frac{1 + \delta}{1 + \epsilon} \right)^3}{3V_p}, \quad (11)$$

where x is the fraction of impurity atoms per one intrinsic defect; $x \leq 2$, $\gamma_v \leq 0.5$.

The following data were used in the calculations: $V_p = 7.4 \times 10^{-2} \text{ nm}^3$ (Cu_2O); $\sigma = 150 \text{ erg/cm}^2$ (Cu_2O); $\mu = 4.8 \times 10^{10} \text{ Pa}$; $\delta = 0.3$; $\epsilon = 0.15$; $\gamma_i = 0.4$; $\gamma_v = 0.1$; $x = 1.5$; $\delta_{\text{Cu}_2\text{O}} = 0.3615 \text{ nm}$; $C_O^{\text{eq}} = 10^{18} \text{ cm}^{-3}$; $D_O = 1.14 \times 10^{-6} \exp(-62500/RT) \text{ m}^2/\text{s}$; $D_v = 0.13 \times \exp\left(-\frac{2.05}{kT}\right)$ [20–23].

The algorithm for solving the problem of modeling the growth and dissolution of oxygen precipitates due to the interaction of point defects in the process of cooling the crystal from the crystallization temperature is based on the use of a monotonic explicit difference scheme of the first order of accuracy for Fokker–Planck equations (9).

The dependencies of the critical radius of oxygen precipitates (Fig. 1) show that near the crystallization front (at $T = 1357 \text{ K}$), the size of the critical oxygen precipitate nucleus is 0.15 nm. The minimum values $n_O^{\text{cr}} = n_O^{\text{cr},0} \approx 311$ are reached in the initial state at $T = 1357 \text{ K}$ and increase with decreasing temperature. An increase in the critical radius of precipitates during crystal cooling leads to a decrease in their growth rate and, accordingly, a decrease in the precipitation rate.

Figure 2 shows the simulation of the kinetics of precipitation upon cooling of a growing crystal according to an exponential law in the temperature

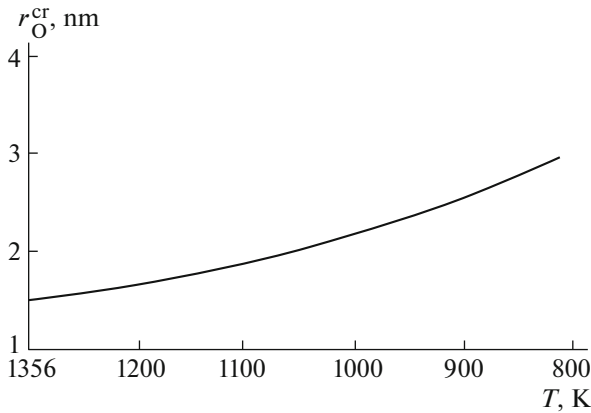


Fig. 1. Dependence of the critical radius of the oxygen precipitate on temperature when the crystal is cooled after growth.

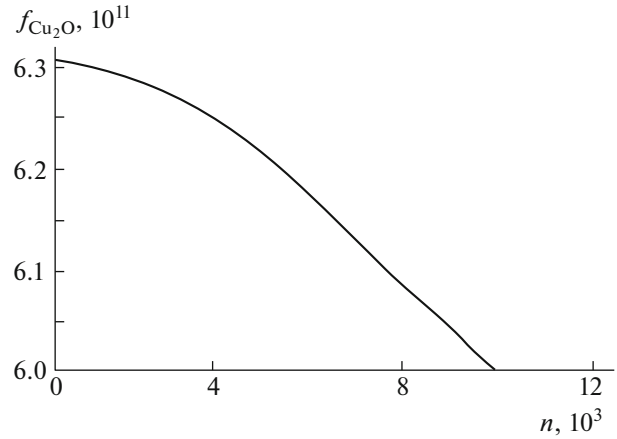


Fig. 2. Size distribution function of oxygen precipitates $f_{Cu_2O}(n)$ during crystal cooling after growth.

range from 1357 to 1403 K. It is assumed that the concentration of nucleation centers for oxygen precipitates is $\sim 10^{12} \text{ cm}^{-3}$.

PROBABILISTIC APPROACH

In Vlasov’s model, the periodic structure of crystals is due to the specifics of the statistical laws of particle motion that correlate the periodic structure with the freedom of movement of atoms rather than a consequence of restrictions on the freedom of movement of atoms through a crystal. Therefore, the probability of meeting an atom in interstices is always nonzero [7, 24]. The model is based on the solution of Vlasov’s kinetic equation, which is a system of equations describing the evolution of a continuum of particles with a pair interaction potential [25]. The solution of this equation under certain conditions leads to the description of the ideal periodic structure of the crystal [24].

Vlasov’s model is based on the following basic physical provisions [24]: (1) the rejection of the principle of spatial and velocity localization of particles (in terms of classical mechanics), which takes place regardless of force interactions; (2) the introduction of force interactions by analogy with classical mechanics but taking into account the new principle of nonlocalization of particles; (3) the description of the behavior of each particle of the system using the f -function extended in the phase space. This approach combines the concepts of continuity and corpuscularity, since the original way of describing the motion of a particle is associated with an extended function, and the point character of a particle manifests itself only in a particular case [26].

In the general case, Vlasov’s equation describes the evolution of the distribution function $f(x, v, t)$ of the

continuum of interacting particles in Euclidean space in terms of velocity and coordinate at time t ,

$$\frac{\partial f}{\partial t} + \left(\frac{\partial f}{\partial x}, v\right) + \left(\frac{\partial f}{\partial v}, F\right) = 0, \tag{12}$$

$$F = -\frac{\partial}{\partial x} \int K(x, y) f(y, v, t) dv dy,$$

where K is the pair interaction potential, which in real problems depends on the distance $|x - y|$, and F is the total force with which all particles act on one of them, which is at point x at time t [25]. To distinguish the types of interactions, the systems of Vlasov equations are usually discussed (Vlasov–Poisson, Vlasov–Maxwell, Vlasov–Einstein, and Vlasov–Yang–Mills equations [26]).

To describe the stationary properties of a crystal, the concept of particle distribution density $\rho(r) = \int f(r, v) dv$ is used. The molecular field is determined only by the probable positions of atoms rather than by their exact positions, which is expressed by a potential function containing the probability density of particles, taking into account the temperature distribution of particles [24]. The selection of the pair interaction potential depends on the problem under consideration. Then, the nonlocal model of a crystal is based on the following nonlinear equations, which make it possible to calculate the molecular potential and density of particles under conditions of temperature equilibrium [24]:

$$V(r) = \lambda k T \int_{-\infty}^{\infty} K_{1,2}(r) \exp\left(-\frac{K_{1,2}(r)}{kT}\right) dr, \tag{13}$$

$$\rho(r) = \lambda k T \exp\left(-\frac{K_{1,2}(r)}{kT}\right),$$

where k is a Boltzmann constant; $K_{1,2}$ is a potential for pair interaction; λ is some characteristic number. The

initial equations are those for two particles under stationary conditions ($\frac{\partial}{\partial t} = 0$) [7]. Here, the characteristic number is understood as such values of a certain parameter λ , for which Eqs. (13) have solutions that are different from trivial ones [7]. If we take the position of one of the particles as the origin of coordinates, we can determine $\rho(0) = \lambda kT$ [7]. Determining the characteristic numbers in Vlasov's model for solids is essential.

The characteristic number λ can be determined from the main criterion for the existence of a crystalline state, and the crystallization condition can be written as

$$\frac{4\pi N}{kT_m} \int_0^{\infty} K_{1,2}^*(\rho) \rho^2 d\rho = 1, \quad (14)$$

where N is the number of particles; T_m is the melting (crystallization) temperature; $K_{1,2}^* = -K_{1,2}$ [7].

The developed diffusion model of defect formation in covalent crystals is based on the "impurity–intrinsic point defect" interaction upon crystal cooling. We called this process "high-temperature precipitation." It links crystal growth with subsequent heat treatment [1]. The classical approach for metal crystals supposes that high-temperature precipitation also takes place in such crystals. Let us now consider the possibility of the formation of "impurity–intrinsic point defect" complexes near the crystallization front using Vlasov's model.

We estimate the possibility of the formation of stable complexes and the evolution of their distribution density depending on the nucleation temperature in the temperature range from $T_m = 1357$ K to $T = 300$ K. Using the classical approach, it was determined that copper–oxygen complexes form in this temperature range. Consequently, the precipitation process (nucleation, growth, and coalescence of particles of the second phase) occurs over the entire range of cooling temperatures ($T \approx 1357$ – 300 K) after growth.

The interatomic potential gives information about the interaction between copper and oxygen atoms and determines their properties. Model potentials with a small number of parameters are usually considered. This is because functions with a larger number of parameters are obtained based on quantum mechanical calculations, which complicates their analytical consideration. There are various approaches to the calculation of interatomic potentials for materials with metallic bonds. Without dwelling on their analysis, we point out the modified embedded-atom method (MEAM), which is often used for pure metals. Using this method for the "copper–oxygen" system, the value $K_{\min} = 0.78$ eV was obtained [27].

To determine the characteristic numbers of the copper–oxygen complexes (λ), we use Eq. (14) with the number of particles in the complex $N = 2$ and

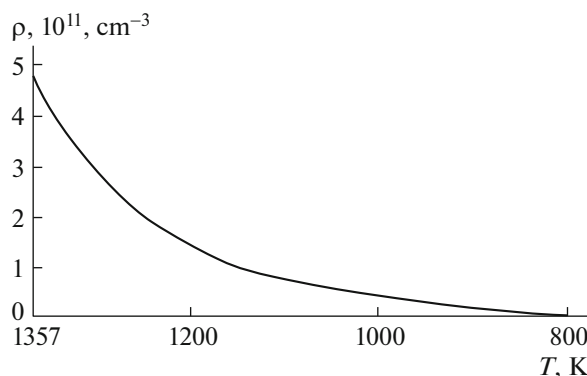


Fig. 3. Temperature dependence of the distribution density of the copper–oxygen complexes.

$K(\rho) = kT \left(1 - e^{-\frac{K_{1,2}}{kT}} \right)$ [7]. The calculation gave $\lambda = 3.319 \times 10^3$ eV $^{-1}$. Based on the fact that the minima of interatomic potentials correspond to a stable equilibrium arrangement of atoms in copper–oxygen complexes, we can determine the distribution density of complexes depending on the crystal cooling temperature $\rho(T) = \lambda kT \exp\left(-\frac{K_{\min}}{kT}\right)$. The evolution of the distribution density upon cooling of a growing crystal is shown in Fig. 3. In this computational experiment, we assumed that the concentrations of nuclei for carbon and oxygen complexes are $\sim 10^{12}$ cm $^{-3}$.

PRELIMINARY (BRIEF) DISCUSSION

Based on the calculation results, we prove that high-temperature precipitation is a process characteristic of both materials with covalent bonds and metal crystals. High-temperature precipitation can cause further defect formation, especially in ultrapure materials. In these crystals, this process is responsible for the formation of secondary structural imperfections, such as dislocation loops, micropores, dislocations, etc. The ease of formation of dislocations in metals masks high-temperature precipitation. However, two independent alternative approaches in solid-state physics confirm the existence of high-temperature precipitation.

The complexity of theoretical calculations is associated with the absence or lack of parameters. This leads to some inaccuracy in the calculations, which can be eliminated by further studies. For example, the role of the effect of self-interstitials on the high-temperature properties of metals is considered in [28].

Despite many years of research on point defects in metals, the issue of their equilibrium concentration remains topical, in particular, in connection with the interstitial theory proposed by Granato [29, 30]. He

proposed an interstitial theory suggesting that the defects responsible for melting are interstitials in a dumbbell-shaped (split) configuration. According to the interstitial theory, the self-interstitials concentration in a crystal near the melting point should be only an order of magnitude lower than the concentration of vacancies. Although this theory offers a qualitative and quantitative explanation for a significant number of essential phenomena observed in liquids and glasses, it has not received wide acceptance. One of the reasons for this is the widely held belief that the concentration of equilibrium dumbbell interstitials is negligible even near the melting point. However, the high-temperature precipitation model can also consider this factor: in such a situation, a joint approach can be used to take into account vacancies and self-interstitials [1].

Of great interest is the use of a probabilistic approach to analyze the formation of a defect structure in crystals with covalent and metallic bonds. In the present work, such an analysis was carried out for metals for the first time. The results correlate perfectly with analogous results for semiconductors [1–4, 8]. Thus, our series of articles prove the validity of Vlasov's theory for solids as applied to real materials, as well as the identity of defect formation in crystals with covalent and metallic bonds.

CONCLUSIONS

This work is one of the first attempts to approach the analysis of the real structure of solids from a unified standpoint. The results of this work indicate that high-temperature precipitation of impurities forms the site of defect formation processes in crystals with covalent and metallic bonds. We can state that Vlasov's assumption about the possibility of describing the real world from a unified standpoint is correct from the point of view of the identity of the results of two alternative theories. The main results are

1. The processes of defect formation upon the growth of dislocation-free covalent and metallic crystals proceed in the same way. They can be described using the diffusion model of the formation of structural imperfections.

2. Using two alternative approaches to describing the defect structure of dislocation-free copper single crystals (the classical theory of the nucleation and growth of particles of the second phase in solids and Vlasov's model for solids), we demonstrated that high-temperature precipitation of impurities occurs when a growing crystal is cooled.

3. High-temperature precipitation of impurities can lead to further development of a defective crystal structure due to the formation of dislocation loops, micropores, dislocations, etc.

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This article is dedicated to the memory of Igor Evgenievich Talanin, the outstanding physicist and materials scientist, professor, doctor of physical and mathematical sciences, and member of the International Union of Crystallographers, who tragically died (December 22, 1952–January 2, 2022). The article was prepared by his son and permanent co-author, Prof. V.I. Talanin. The name of I.E. Talanin is also listed among the authors since he managed to take part in the work.

CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

REFERENCES

1. V. I. Talanin and I. E. Talanin, *The Formation of Structural Imperfections in Semiconductor Silicon* (Cambridge Scholars Publ. Newcastle, 2018).
2. V. I. Talanin and I. E. Talanin, *Phys. Solid State* **58**, 427 (2016).
3. V. I. Talanin, I. E. Talanin, and O. Matsko, *J. Cryst. Growth* **533**, 125472 (2020).
4. V. I. Talanin and I. E. Talanin, *Phys. Status Solidi A* **200**, 297 (2003).
5. M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Clarendon, Oxford, 1954).
6. J. W. Cristian, *The Theory of Transformations in Metals and Alloys* (Pergamon, London, 1965).
7. A. A. Vlasov, *Theory of Many Particles* (Gostekhizdat, Moscow, 1950) [in Russian].
8. V. I. Talanin and I. E. Talanin, *Crystallogr. Rep.* **64**, 550 (2019).
9. Z. Rdzawski, J. Sobota, J. Stobrawa, and W. Głuchowski, *Arch. Metall. Mater.* **59**, 649 (2014).
10. Yongfeng Geng, Yijie Ban, Bingjie Wang, et al., *J. Mater. Res. Technol.* **9**, 11918 (2020).
11. A. Chbihi, X. Sauvage, and D. Blavette, *Acta Mater.* **60**, 4575 (2012).
12. S. Sajadi, S. Hocker, and A. Mora, et al., *Phys. Status Solidi B* **254**, 1600407 (2016).
13. V. G. Babkin, A. I. Trunova, and A. I. Cherepanov, *Russ. Metall.* **2016**, 419 (2016).
14. D. E. Ovsienko, *Origin and Growth of Crystals from Melt* (Kiev, 1993) [in Russian].
15. C. H. Sworn and T. E. Brown, *J. Cryst. Growth* **15**, 195 (1972).
16. H. Fehmer and W. Uelhoff, *J. Cryst. Growth* **13–14**, 257 (1972).
17. I. K. Zasimchuk, D. E. Ovsienko, and A. V. Fomin, *J. Cryst. Growth* **52**, 376 (1981).
18. S. Senkader, J. Esfandyari, and G. Hobler, *J. Appl. Phys.* **78**, 6469 (1995).

19. J. Vanhellefont, *J. Appl. Phys.* **78**, 4297 (1995).
20. H. Magnuson and K. Frisk, Rapport (Inst. Metallforskning, Sweden, 2014).
www.diva-portal.org/smash/record.jsf?pid=diva2:973212
21. D. B. Bulrymowics, J. R. Manning, and M. E. Read, *J. Phys. Chem. Ref. Data* **2**, 643 (1973).
22. G. Neumann and C. Tuijn, *Self-Diffusion and Impurity Diffusion in Pure Metals: Handbook of Experimental Data* (Elsevier, Oxford, 2009).
23. D. Bartdorff, G. Neumann, and P. Reimers, *Philos. Mag. A* **38**, 157 (1978).
24. A. A. Vlasov, *Nonlocal Statistical Mechanics* (Nauka, Moscow, 1978) [in Russian].
25. V. V. Kozlov, *Nonlin. Dyn.* **6**, 489 (2010).
26. V. V. Vedenyapin, *Kinetic Equations of Boltzmann and Vlasov* (Fizmatlit, Moscow, 2001) [in Russian].
27. M. I. Baskes, *Phys. Rev. B* **46**, 2727 (1992).
28. V. Khonik and N. Kobelev, *Metals* **9**, 605 (2019).
29. A. V. Granato, *Phys. Rev. Lett.* **68**, 974 (1992).
30. A. V. Granato, *Eur. Phys. J. B* **87**, 18 (2014).

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