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Molecular dynamics simulation of diffusion along general high-angle grain boundaries in copper and vanadium

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Abstract: In this paper, atomistic simulations were used to calculate the characteristics of grain boundary diffusion, estimation of which from the results of experimental studies is limited. The methods for specifying interatomic interactions, constructing model samples, and processing the results of molecular dynamics simulations for calculation of grain boundary diffusion coefficients in accordance with those determined from the results of diffusion experiments in polycrystals are discussed and new approach is proposed. The proposed approach is illustrated on the example of molecular dynamics simulations of general high-angle grain boundaries in copper and vanadium. On the example of copper, a good agreement between calculated within our approach and experimental grain boundary diffusion characteristics was demonstrated. For vanadium, a theoretical prediction of temperature dependence of product of its grain boundary self-diffusion coefficient on the effective grain boundary width is given.

Keywords: grain boundaries, diffusion, molecular dynamics, copper, vanadium

1. Introduction

Grain boundary (GB) diffusion in polycrystalline metals and alloys is an important process controlling grain boundary segregation, high-temperature creep by the Cobble mechanism, and other phenomena controlled by GB diffusion [1]. The main characteristic of this process is a GB diffusion coefficient D_{GB} which can be established from the results of diffusion experiments in polycrystals [2, 3]. At the same time, experimental research in this direction is quite a difficult task and is represented by a relatively small number of papers. Series of papers (reviews [4, 5, 6] and references therein) are devoted to the study of GB diffusion in polycrystalline metals. One of the determining reasons for the limited number of experimental studies is the growth of grains during diffusion experiments [7] which are needed to be conducted at sufficiently high temperatures to obtain representative experimental data. Also, residual impurities of elements, which are present even in high-purity metals, have a hardly predictable effect on diffusion characteristics due to GB segregation. For example, the results of various diffusion experiments show a significant variation in the values of the diffusion activation energy in copper ranging from 72.5 to 120 kJ/mol [8]. In the case of vanadium, we do not know any experimental data on the GB diffusion.

To obtain the missing information on diffusion characteristics, molecular dynamic (MD) simulation can be used. The MD method is formally accurate at temperatures

above the Debye temperature and correctly take into account the effects of anharmonicity. In the last decade, theoretical studies in this direction have been actively carried out for face-centered cubic (FCC) and body-centered cubic (BCC) metals and their alloys [9,10,11,12,13], including high-entropy alloys [11,12]. At the same time, authors of these works face with certain difficulties related to obtaining and interpreting the results of MD simulations for comparison with the results of diffusion experiments.

Obtaining reliable quantitative information about GB diffusion imposes a number of requirements on atomistic simulation methods, including specifying interatomic interactions, constructing model samples with GB, and processing the results of MD simulations to obtain diffusion characteristics of GB in accordance with the physical meaning of these characteristics from experimental studies. To date, MD simulations of flat GBs (without triple junctions) are carried out on samples constructed within the coincidence site lattice (CSL) model [9,10,11,12,13,14,15]. The current problem in interpreting the results of MD simulations for comparison with diffusion experiments is ambiguous use of the Einstein-Smolukhovskiy relation to obtain the coefficients of GB diffusion. In one approach, an artificial separation of atoms in the GB region from atoms in the bulk grain is introduced to substitute their number in the Einstein-Smolukhovskiy ratio [10,12,13,15]. In another approach, only diffusion displacements in the plane of the GB are taken into account and a two-dimensional diffusion coefficient is calculated,

which is taken as the GB diffusion coefficient [12]. At the same time, in the Fisher model [16], the GB diffusion coefficient D_{GB} , determined from diffusion experiments in polycrystals, is the volume diffusion coefficient in the GB phase. Thus, it is currently relevant to develop and test atomistic simulation methods for reliable quantitative prediction of the GB diffusion coefficients D_{GB} , primarily in pure metals, in accordance with D_{GB} , determined from the results of diffusion experiments in polycrystals. After a reliable justification, these methods can be further developed for the case of alloys.

In this work, we propose an approach for the reliable prediction of self-diffusion coefficients in the lattices of both FCC and BCC metals based on MD simulations with interatomic potentials constructed within the N -body method [17,18,19,20]. For a detailed presentation of the proposed approach, we justify the choice of N -body interatomic potentials, construct the model samples with general high-angle GBs, analyze the results of MD simulations conducted with chosen interatomic potentials and model samples, and compare the absolute values of GB diffusion characteristics in copper with experimental data at particular temperatures. In the case of vanadium, we offer the calculated GB diffusion coefficients as a theoretical prediction filling the gap in experimental data for GB diffusion in this metal. Also, we compare the calculated coefficients of grain boundary self-diffusion D_{GB} with the coefficients of bulk self-diffusion D_b and the known results of diffusion experiments in the considered metals.

2. Methods

The reliability of theoretical predictions using MD simulations is primarily determined by the quality of specifying interatomic interactions within the Born-Oppenheimer approximation. Within this approximation, the electron subsystem adiabatically follows the displacements of ions, and the positions of the latter determine the coordinates of atoms. The interactions between atoms are given by the dependence of the effective potential energy of the system on their coordinates.

To date, a number of methods have been developed for specifying interatomic interactions, which make it possible to consistently increase the accuracy until a formally accurate result is achieved, which should not depend on the method used. Among the methods that have this property, we note the methods based on the density functional theory (DFT) [22,23], the method of decomposition into a series of N -body interactions [17] and the method of artificial neural networks (ANN) [24]. The advantage of DFT methods is the ability to predict the characteristics of materials without using adjustable parameters (*ab initio* or from first principles). At the same time, due to the unknown exact type of the electron density functional, the DFT contains errors associated with the model assignment of the exchange-correlation energy (usually local density approximation, LDA, or generalized-gradient approximation, GGA), which leads to significant errors for metals with large gradients of valence electron density [25,26]. Modern ANN methods use only DFT data to build their training databases, therefore they inherit the DFT errors noted above. The N -body method, based on a formally exact

decomposition into a series of N -body interactions, allows one to exactly take account for 3-body interactions while using a centrally symmetric approximation for specifying an infinite series of multiparticle interactions (starting from 4-body interactions). However, in contrast to ANN, N -body method uses as a training database both a large set of DFT calculation results as well as experimental data using a procedure to reduce the discrepancy between these two types of data. The simultaneous use of DFT and experimental data to optimize the parameters of potentials was proposed in [27] for the first time. The DFT data ensure the transferability of N -body potentials to atomic configurations that are not used to optimize potential parameters, while the experimental data increase the accuracy of predicting the atomic characteristics of metals and alloys in comparison with the DFT method.

On the example of several d-metals, it is shown that within the framework of the accepted approximation, interatomic potentials constructed within the N -body method predict a number of properties of d-metals in a good agreement with experimental values, including melting temperature, thermal expansion and vacancy characteristics [17,18,19,20,21]. Accurate reproduction of these properties by interatomic potentials is of decisive importance in the accuracy of the prediction of diffusion characteristics at specific temperature values. For comparison, ANN reproducing a large sample of DFT data with high accuracy, for example, predicts the value of $T_m = 3000$ K for the melting temperature of Ta, which is 293 K lower than the experimental value of 3293 K [28]. It is obvious that in addition to the problem of the accuracy of the prediction of the values of the diffusion coefficients, the study of diffusion processes in the BCC crystal lattice Ta above the temperature 3000 loses its physical meaning when using the marked ANN potential for Ta. At the same time, in the case of N -body interatomic potential, the predicted value of melting temperature for Ta is $T_m = 3291$ K, along with a good agreement of a wide range of N -body characteristics of tantalum with experimental data [29]. Also for vanadium, the melting temperature $T_m = 2181$ K calculated using the N -body potentials is close to the experimental value $T_m = 2183$ K [17]. The high reliability of the predicted thermal expansion, melting temperature, and vacancy energy, along with elastic constants, dispersion curves of phonons, and number of other atomic characteristics, justifies the use of vanadium N -body potentials [17] for the quantitative prediction of the GB diffusion characteristics in this metal. In this regard, we will further consider the construction of model samples containing GB in a BCC metal lattice for the implementation of the noted prediction by atomistic simulation methods.

The bicrystal model constructed within the framework of the coincidence site lattice (CSL) model is widely used for the simulation of GBs [10,11,12,14,15]. In this case, the model sample contains a GB with a given value of the inverse density of coinciding sites Σ and is convenient for simulation by the MD method using periodic boundary conditions. However, most GBs in polycrystalline metals are general high-angle GBs. Such GBs are characterized by the absence of a CSL. In this case, the inverse density of coinciding sites Σ formally tends to infinity. In this regard, in this paper we use the method of constructing model samples of the general GB proposed and tested in [30] on the example of studying GB

diffusion in the Nb-Cu system. The advantage of this method is that it allows obtaining a sample using periodic boundary conditions in three orthogonal directions. In this case, the sample does not contain any other defects of the crystal lattice (e.g., triple junctions and vacancies), except GBs.

For MD simulations of GB diffusion we constructed several model samples using the approach described above. The model sample of vanadium V_1 has rectangular form and contains 74 000 atoms in the simulation cell, see Fig. 1. Sizes of the V_1 sample are 8 × 8 nm in the GB plane and 16 nm in the normal direction to the GB plane. The atomic structure of the V_1 sample is illustrated in Fig. 1 and represented by two bulk grains with bcc lattice without defects divided by two general high-angle GBs due to periodic boundary conditions. The nearest neighbor analysis implemented in the OVITO software package was used to visualize the atomic structure in the constructed sample [31]. In Fig. 1, the blue color denotes atoms with a local BCC lattice environment, while the gray color denotes atoms belonging to the grain boundary region.

For investigation of dependence of the MD simulation results on the sizes of model sample we constructed yet another vanadium sample V_2 with sizes of 4 × 4 × 11 nm containing 10 288 atoms in the simulation cell. The common view of the model sample of Cu is illustrated in work [20]. The reciprocal densities of coinciding sites Σ , grain boundary energies γ_{GB} and grain boundary volumes V_{GB} related to unit GB area of two constructed samples of V are presented in Table 1 in comparison with GB characteristics of Cu [20].

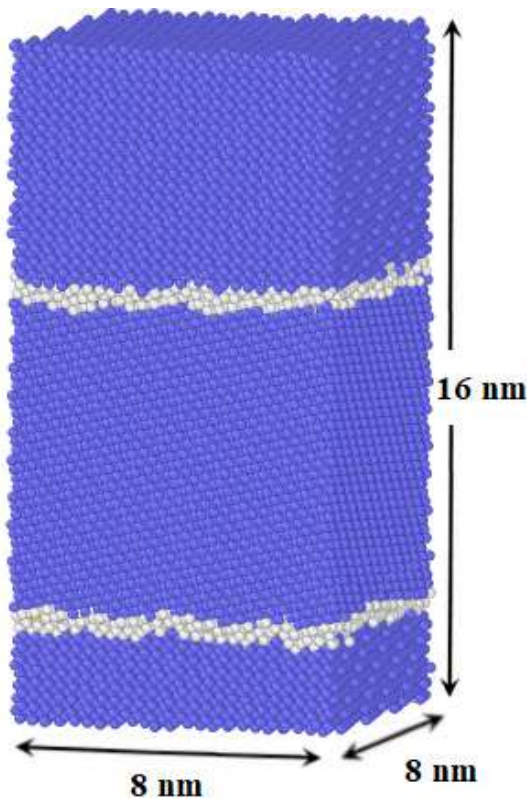


Fig. 1. (Color online) The simulation cell of the model sample V_1 with orthogonal shape, containing two grain boundaries. Periodic boundary conditions are given in three orthogonal directions. The blue color denotes atoms with a local BCC lattice environment, while the gray color denotes atoms belonging to the grain boundary region.

Table 1. Grain boundary energy γ_{GB} (J/m²), grain boundary excess volume V_{GB} (Å), and reciprocal density of coinciding sites Σ in the model specimens of Cu and V.

Specimen	γ_{GB}	V_{GB}	Σ
Cu [20]	0.87	0.21	10^3
V_1	1.39	0.17	10^3
V_2	1.30	0.15	200

To estimate the magnitude of Σ we used the reciprocal value of relation of area per atom in the most close-packed crystallographic plane of the body-centered cubic (BCC) lattice of vanadium $S_{at}^{[110]}$ to the GB area S_{GB} .

As can be seen from the data presented in Table 1, two different vanadium samples, significantly differing in size and Σ , have very similar values of the characteristics of GB in accordance with the properties of general high-angle GB. This implies that sizes and reciprocal density of coinciding sites Σ (of order of 10^3) in the V_1 sample are sufficient for effective simulation of general GB. Also, in the future, the coincidence of the GB diffusion characteristics in V_1 and V_2 samples will be noted. It is interesting to note here that the ratio of the energies of the general GB in vanadium and copper, 1.60 (V_1) and 1.49 (V_2), practically coincides with the value of 1.50 of the ratio of the sublimation energies of these metals (5.31/3.54). The constructed samples, which effectively represent the general GB, allow us to study the GB diffusion without artificially specifying vacancies or interstitial atoms. As it was shown in [30] on the example of copper modeling, the structure of a general GB provides the implementation of GB diffusion without additional assignment of defects.

The characteristics of GB diffusion determined from diffusion experiments in polycrystals are the parameters of the GB model as a homogeneous GB phase of a certain thickness δ , characterized by a diffusion coefficient D_{GB} [2, 3]. In this case, the Einstein–Smolukhovsky relation which is used for calculation of diffusion coefficients D_b in the volume of grains from the results of MD simulation of diffusive displacements of atoms leads to the problem of ambiguous choice of atoms in GB. Without such a choice, the value of the root-mean-square displacement of atoms tends to zero with an increase in the size of the calculation cell and a corresponding increase in the contribution of the grain volume to the sum of the squares of the diffusion displacements of atoms. At the same time, even the choice of GB atoms does not allow to obtain exactly D_{GB} , but only the activation energy of GB diffusion from the results of MD simulation for a series of temperatures. In this paper we use the analytical expression [30]

$$(D_{GB} - D_b)\delta = \Omega \zeta_{GB} / 6, \quad (1)$$

where D_{GB} — GB diffusion coefficient, D_b — bulk diffusion coefficient, δ — effective GB thickness, and Ω — atomic volume. Relation (1) binds the parameters D_{GB} and δ which are determined from the results of diffusion experiments and the rate of increase of the excess of the sum of squares of the diffusion displacements of atoms in the simulation cell ζ_{GB} , associated with the grain boundaries and attributed to the unit area of these boundaries [30]. The value of ζ_{GB} at the specified temperature T is determined from MD simulation as the slope (ζ/t) of dependence of the sum of squared diffusion displacements of atoms $\zeta(t)$ in the

simulation cell on the simulation time t . Dividing the slope (ζ/t) on the grain boundary area S_{GB} in the simulation cell one can get $\zeta_{GB} = (\zeta/t)/S_{GB}$. Here we suppose that the sum of $\zeta(t)$ is equal to the excess attributed to the GB since diffusion displacements do not occur in the volume of grains without GB due to the absence of vacancies in the initial model samples. Next, the value of the product $D_{GB}\delta(T)$ is calculated from the formula (1). At the same time $D_b\delta(T)$ is assumed to be zero due to the absence of bulk diffusion in the simulated sample, as discussed above. It should be noted here that from the results of diffusion experiments it is also possible to determine only the product of parameters $D_{GB}\delta(T)$ [2, 3], except for the special case of diffusion in C regime, according to the classification of Harrison [2, 3]. In this case, the GB diffusion coefficient D_{GB} is determined by dividing the obtained value of the product by the effective width δ . The assumption that $\delta = 5 \text{ \AA}$, introduced by Fisher [16], is a good approximation and agrees with experimental estimates of the width of the GB by high-resolution electron microscopy [2, 3], as well as with the analysis of a series of experimental studies on the GB diffusion in B and C regimes performed by Divinski and Bokstein [32].

As can be seen from relation (1), in atomistic simulations, the product $D_{GB}\delta$ has physical meaning of ζ_{GB} value up to a multiplier. This value is determined by the excess of the additive value — the sum of the squares of the diffusion displacements of atoms, therefore it is determined unambiguously. Also, it is the excesses of additive quantities (volume, Gibbs energy, and others) that are uniquely determined by the characteristics of GB.

3. Results and discussion

To obtain the sum of the squares of diffusion displacements of atoms $\zeta(t)$ in the simulation cell, we performed MD simulation of the NPT ensemble of vanadium model samples V_1 and V_2 in the temperature ranges 1500–2100 K and 1300–2100 K with increment of 100 K, respectively. The lower temperature limit is determined by the limitation of

the MD method, and the upper limit was determined by the melting point of vanadium 2181 K, calculated using the N -body interatomic potential for vanadium [17]. For each MD temperature, the simulation was carried out for 3 ns and atomic configurations were recorded every 50 ps.

Calculated values of the sum of squares of diffusion displacements of atoms $\zeta(t)$ from the simulation time t for the chosen for the selected range of temperatures and the coefficients of GB diffusion D_{GB} are presented in Fig. 2. For comparison, Fig. 2 also presents the values of the bulk diffusion coefficients D_b and GB diffusion coefficients in copper, calculated using the same method described above, along with the results of well-known diffusion experiments in copper and vanadium.

As can be seen from Fig. 2 a, the calculated dependences of the sum of the squares of the diffusion displacements of atoms $\zeta(t)$ for the model sample V_1 are linear in nature and ζ increases monotonically with increasing temperature. This indicates the typical behavior of the diffusion process of displacements of atoms in the general GB, usually observed during diffusion in the volume of grains of metals and alloys. At the same time, the coefficients of GB diffusion in samples V_1 and V_2 coincide, which, along with the agreement of the energy and the volume of the GB in these samples, confirms the sufficiency of the value $\Sigma = 10^3$ in the model sample for the study of the properties of the general GB.

Experimental data for GB and bulk self-diffusion for a number of metals were analyzed by Bokstein and Rodin [4], Ashby and Brown [6], Gust et al. [5], and empirical correlations have been established. The magnitude of GB self-diffusion coefficients is 4–8 orders of magnitude greater than that of bulk self-diffusion coefficients, depending on temperature [3]. This difference in the self-diffusion coefficients is due to the difference in activation energies, and for BCC and FCC metals the E_{GB}/E_b ratio is 0.57 and 0.49, respectively [5]. The pre-exponential multipliers for BCC and FCC metals are close to each other and the value of $D_{GB}\delta(T)$ tends to be $2.8 \times 10^{-18} \text{ m}^3/\text{s}$ and $1.1 \times 10^{-18} \text{ m}^3/\text{s}$ at the melting temperature [5]. Figure 2 shows that for both vanadium and copper the GB

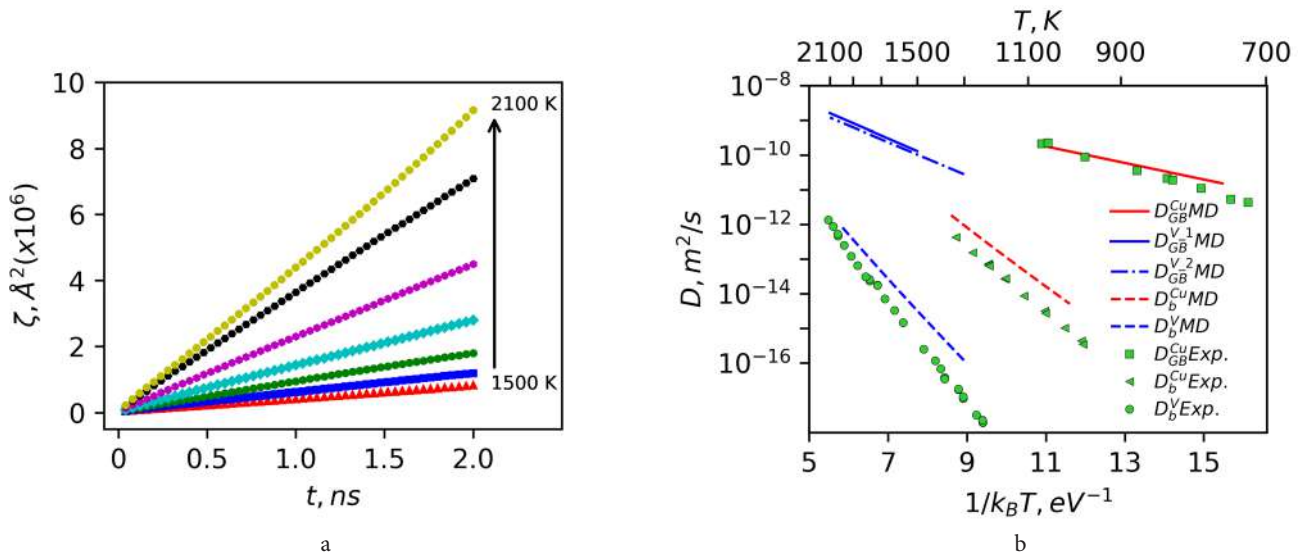


Fig. 2. (Color online) Sums of squares of diffusion displacements of atoms ζ in the sample V_1 (a). Coefficients D of bulk and GB diffusion in copper and vanadium as functions of $1/k_B T$, where k_B is the Boltzmann constant. The calculated values (MD) computed by us earlier for D in V and Cu are published in the works [20, 21]. Experimental values (Exp) are taken from the works [8, 33, 34] (b).

diffusion coefficients are several orders of magnitude higher than their counterparts in the grain volume. This agrees with modern understanding and experimental data on GB self-diffusion about the higher rate of diffusion processes in GB [1, 3, 4, 5, 6, 35]. The ratio of calculated activation energies of GB and bulk self-diffusion is 0.39 for vanadium, and 0.28 for copper. The calculated ratios of activation energies of GB and bulk self-diffusion for copper and vanadium have a systematic underestimation, but qualitatively agree with empirical dependences [5]. For BCC metals the value of E_{GB}/E_b ratio is larger than that for FCC metals. It should also be noted that the value of the ratio of experimentally determined activation energies of self-diffusion E_{GB}/E_b for copper decreases with increasing purity of the studied samples from 0.43 to 0.37, for samples of purity 5N and 5N8, respectively [4]. The value of the activation energy ratio in copper of 0.28 obtained by us corresponds to the tendency to decrease the value of E_{GB}/E_b with increasing purity of copper, since the model samples in our work contain only copper atoms. The obtained values of $D_{GB}\delta(T)$ at melting temperatures of 2183 K for vanadium and 1356 K for copper are $1.1 \times 10^{-18} \text{ m}^3/\text{s}$ and $3.4 \times 10^{-19} \text{ m}^3/\text{s}$. For vanadium, the value of $D_{GB}\delta(T)$ at melting temperature is in quantitative agreement with the established empirical dependence for BCC metals [5]; in the case of copper, the calculated value of $D_{GB}\delta(T)$ is overestimated by one order of magnitude.

The above mentioned correlations of diffusion characteristics for copper and vanadium are in good agreement with those established from the analysis of experimental data. At the same time, the theoretical prediction of D_{GB} coefficients agrees well with the experimental data in the case of high-purity copper [8]. The coincidence of the results of independent computer and real diffusion experiments confirms the reliability of each of these results. For vanadium, the results of real diffusion experiments for establishing the GB diffusion characteristics are absent. In this regard, a theoretical prediction of the diffusion characteristics of GB in vanadium, obtained using carefully validated atomistic simulation methods, is of great importance. For convenience of further use, we present the predicted results in the form of a numerical Arrhenius-type dependence

$$D_{GB}\delta(T) = (4.33 \pm 0.32) \cdot 10^{-16} \times \exp(-(1.13 \pm 0.05)\text{eV}) / (k_B T), \text{ m}^3/\text{s} \quad (2)$$

This dependence includes the pre-exponential factor and the activation energy of self-diffusion, where the absolute values of temperature T are given in Kelvins. To obtain D_{GB} from the ratio (2), we assume the effective diffusion width of grain boundaries $\delta = 5 \text{ \AA}$, as it is justified and accepted in the literature.

4. Conclusion

A detailed discussion of atomistic simulation methods for a reliable quantitative prediction of the diffusion characteristics of grain boundaries in accordance with those characteristics determined from the results of diffusion experiments in polycrystals at specific temperature values has been carried out. In this regard, special attention is paid to general high-angle grain boundaries. Using the example of self-diffusion in

copper, it is shown that a well-founded theoretical prediction makes it possible to increase the reliability of the results of experiments to establish the characteristics of GB, which may be limited due to the complexity of experimental techniques and the difficult-to-control effect of residual impurities. From the results of molecular dynamic simulations, the temperature dependence of the self-diffusion coefficient in the vanadium grain boundaries was established for the first time. The described approach can be used for quantitative prediction of diffusion characteristics in alloys, however, in this case, the methods of atomistic simulation should be supplemented by consideration of grain boundaries segregations. Research in this direction is being conducted. The development and use of methods for the quantitative theoretical determination of diffusion characteristics opens the possibility of establishing model parameters for predicting processes in metals and alloys controlled by grain-boundary diffusion, such as creep by the Coble mechanism.

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References

1. Y.R. Kolobov. Diffusion-Controlled Processes at Grain Boundaries and Plasticity of Metallic Composite. Novosibirsk, Nauka (1998). 184 p. (in Russian)
2. I. Kaur, Y. Mishin, W. Gust. Fundamentals of Grain and Interphase Boundary Diffusion. 3rd edn. Chichester, Wiley (1995) 536 p.
3. P. Heitjans, J. Kärger. Diffusion in condensed matter: methods, materials, models. New York, Springer Science & Business Media (2005) 955 p.
4. B. Bokstein, A. Rodin. Diff. Found. 1, 99 (2014). [Crossref](#)
5. W. Gust, S. Mayer, A. Bögel, B. Predel. J. Phys. Colloq. 46 (C4), 537 (1985). [Crossref](#)
6. A.M. Brown, M.F. Ashby. Acta Metall. 28 (8), 1085 (1980). [Crossref](#)
7. M. Köppers, Y. Mishin, C. Herzig. Acta Metall. Materialia. 42 (8), 2868 (1994). [Crossref](#)
8. T. Surholt, C. Herzig. Acta Mater. 45 (9), 3817 (1997). [Crossref](#)
9. I.I. Novoselov, A.Y. Kuksin, A.V. Yanilkin. Phys. Solid State. 56, 1025 (2014). [Crossref](#)
10. V.V. Popov, M.E. Stupak, M.G. Urazaliev. JPED. 43 (4), 401 (2022). [Crossref](#)
11. F. Junhong, Z. Weiqiang. Phys. Scr. 98 (3), 035006 (2023). [Crossref](#)
12. A. Seoane, D. Farkas, X.M. Bai. J. Mater. Sci. 58, 8845 (2023). [Crossref](#)
13. S. Starikov, M. Mrovec, R. Drautz. Acta Mater. 188, 560 (2020). [Crossref](#)
14. M.R. Sørensen, Y. Mishin, A.F. Voter. Phys. Rev. B. 62 (6), 3658 (2000). [Crossref](#)
15. I. Chesser, Y. Mishin. Commun. Mater. 3 (1), 90 (2022). [Crossref](#)
16. J.C. Fisher. J. Appl. Phys. 22 (1), 74 (1951). [Crossref](#)
17. A.G. Lipnitskii, V.N. Saveliev. Comput. Mater. Sci. 121, 67 (2016). [Crossref](#)

18. V.N. Maksimenko, A.G. Lipnitskii, V.N. Saveliev, I.V. Nelasov, A.I. Kartamyshev. *Comput. Mater. Sci.* 198, 110648 (2021). [Crossref](#)
19. V.N. Maksimenko, A.G. Lipnitskii, A.I. Kartamyshev, D.O. Poletaev, Y.R. Kolobov. *Comput. Mater. Sci.* 202, 110962 (2022). [Crossref](#)
20. A.I. Kartamyshev, A.G. Lipnitskii, V.N. Maksimenko, A.V. Vyazmin, I.V. Nelasov, D.O. Poletaev. *Comput. Mater. Sci.* 228, 112284 (2023). [Crossref](#)
21. A.I. Kartamyshev, A.G. Lipnitskii, V.N. Saveliev, V.N. Maksimenko, I.V. Nelasov, D.O. Poletaev. *Comput. Mater. Sci.* 160, 30 (2019). [Crossref](#)
22. R. Car, M. Parrinello. *Phys. Rev. Lett.* 55 (22), 2471 (1985). [Crossref](#)
23. W. Kohn, L.J. Sham. *Phys. Rev.* 140 (4A), 1133 (1965). [Crossref](#)
24. Y. Mishin. *Acta Mater.* 214, 116980 (2021). [Crossref](#)
25. K. Lejaeghere, J. Jaeken, V. Van Speybroeck, S. Cottenier. *Phys. Rev. B.* 89 (1), 014304 (2014). [Crossref](#)
26. K. Lejaeghere, V. Van Speybroeck, G. Van Oost, S. Cottenier. *Crit. Rev. Solid State Mater.* 39 (1), 1 (2014). [Crossref](#)
27. Y. Mishin, D. Farkas, M. J. Mehl, D. A. Papaconstantopoulos. *Phys. Rev. B.* 59 (5), 3393 (1999). [Crossref](#)
28. Y.S. Lin, G.P.P. Pun, Y. Mishin. *Comput. Mater. Sci.* 205, 111180 (2022). [Crossref](#)
29. D.O. Poletaev, A.G. Lipnitskii, V.N. Maksimenko, Y.R. Kolobov, A.G. Beresnev, M.S. Gusakov. *Comput. Mater. Sci.* 216, 111841 (2023). [Crossref](#)
30. A.G. Lipnitskii, I.V. Nelasov, Y.R. Kolobov. *DDF.* 309–310, 45 (2011). [Crossref](#)
31. A. Stukowski. *Model. Simul. Mat. Sci. Eng.* 18 (1), 015012 (2009). [Crossref](#)
32. S.V. Divinski, B.S. Bokstein. *DDF.* 309–310, 1 (2011). [Crossref](#)
33. J. Pelleg. *Philos. Mag.* 29 (2), 383 (1974). [Crossref](#)
34. D.B. Butrymowicz, J.R. Manning, M.E. Read. *JPCRD.* 2 (3), 643 (1973). [Crossref](#)
35. D. Gupta. *Diffusion processes in advanced technological materials.* Norwich, William Andrew (2005) 532 p. [Crossref](#)