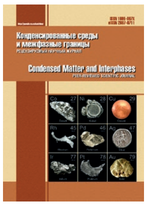
Condensed Matter and Interphases. 2022;24(4): 475–482



ISSN 1606-867X (Print)
ISSN 2687-0711 (Online)
Condensed Matter and Interphases
Kondensirovannye Sredy i Mezhfaznye Granitsy
https://journals.vsu.ru/kcmf/

Original articles

Research article
https://doi.org/10.17308/kcmf.2022.24/10552

Migration of an incommensurate intercrystalline boundary and boundary self-diffusion

V. G. Kul'kov✉

Volzhsk Branch of Moscow Power Engineering Institute,
69 Lenina prospect, Volzhsky 404101, Russian Federation

Abstract

Most grain boundaries found in polycrystalline metals are not special. The angle of their mutual disorientation is an arbitrary value, and the axis of rotation is arbitrarily oriented to the plane of the boundary. Periodic atomic structures such as lattices of coincident nodes, alternating polyhedra, and others do not arise within such boundaries. They are called boundaries of a general type, non-special, arbitrary, or incommensurate. The general theory of relaxation processes at such boundaries has not yet been sufficiently developed. The aim of the study was the development of the model of migration of an incommensurate intercrystalline boundary at the atomic level and the description of the process of self-diffusion along it.

A circle called the main region is described around each boundary lattice node of one of the crystallites. If there is an atom in the node, then an atom of another crystallite is excluded from entering it. In the case of a vacant node in the main region, such an atom can be located. An atom in a planar picture means an atomic series in the three-dimensional case. The distribution of vacant nodes of the growing crystallite is uniform over the flat reduced main region. The migration mechanism involves the implementation of the following main processes: local rearrangement of atomic configurations and self-diffusion of atoms in the transverse direction of the slope axis.

The characteristic times of these processes and the expression for the migration rate were found. The migrating boundary contains a large number of delocalised vacancies. This leads to the high diffusion mobility of atoms. Most vacancies in the boundary are not of thermal origin, but are determined only by the geometric atomic structure of the boundary. In this case, the expression for the boundary self-diffusion coefficient does not contain a multiplier depending on the activation energy of vacancy formation. This leads to the fact that the coefficient of self-diffusion along the migrating boundary is significantly higher than in the stationary boundary. The model of an incommensurate boundary allows us to describe its migration and calculate the self-diffusion coefficient.

Keywords: Incommensurate intercrystalline boundaries, Delocalised vacancies, Boundary self-diffusion, Migration mobility

For citation: Kul'kov V. G. Migration of an incommensurate intercrystalline boundary and boundary self-diffusion. *Condensed Matter and Interphases.* 2022;24(4): 475–482. https://doi.org/10.17308/kcmf.2022.24/10552

Для цитирования: Кульков В. Г. Миграция несоразмерной межкристаллитной границы и граничная самодиффузия. *Конденсированные среды и межфазные границы.* 2022;24(4): 475–482. https://doi.org/10.17308/kcmf.2022.24/10552

✉ Viktor G. Kul'kov, e-mail: vikulkov@yandex.ru

1. Introduction

A large number of various models have been proposed to describe the atomic structure of intercrystalline boundaries in metals and relaxation processes involving them. Among them there is a special class of boundaries. They separate two crystallites mutually rotated for angle at which a lattice of coinciding nodes, common to them, is formed. The atomic structure of such boundaries has a semblance of a crystal structure and is characterised by periodicity. Small deviations from the special misorientation of crystallites are provided by the introduction of grain boundary dislocations. The theory of special boundaries is well developed. However, among the boundaries actually existing in polycrystalline materials, their number is low and, according to various estimates, is approximately one tenth. A significant proportion of boundaries do not correspond to special misorientations. Their atomic structure is formed by conjugation of two surfaces with rational Miller indices whose translation periods in one or two directions are incommensurable, such as, for example, $\sqrt{2}$ and 1. This means that the lengths of such segments cannot be expressed as rational numbers when measured with a ruler with a one scale bar. The imposition of such surfaces excludes the possibility of the appearance of periodic structures in the boundary. Similar structures also appear when noncrystallographic planes of adjacent lattices with Miller indices, some of which are irrational numbers, are conjugated. Grain boundaries of this type are called arbitrary, ordinary, non-special, or incommensurate.

The model of the atomic structure of an incommensurate intercrystalline boundary was successfully used to describe structural rearrangements in the process of intergranular slippage [1]. According to this model, rearrangements of atomic configurations in the near-boundary region occur in the effective potential field that exists in this region and is created by the totality of all near-boundary atoms. The characteristic of the position of each atom is a scalar or vector value, called the mismatch parameter (distance), which uniquely determines its geometric and energy state. It determines the position of each atom of one of the two connecting crystallites with respect to the coordinate system of the other. A somewhat different parameter was introduced to describe the change in the atomic structure of grain boundaries in aluminium and is called the order parameter [2]. For atoms with certain regions of variation of the mismatch parameters, double-well energy configurations with different pit depths are formed in the boundary. The elementary act of sliding is the jump of an atom from one pit to an adjacent deeper pit. The dimensions of such regions depend on the structure of the boundary and the magnitude of the stresses acting in it. The resulting rate of the process is determined by the size of the regions, the value of the activation barrier, and the density of states. Accounting for these factors for boundaries with different types of incommensurability leads to different types of functional relationship between the slip rate and the magnitude of the applied stresses [3]. The development of ideas about incommensurate structures allowed possible to describe not only their energy [4], but also many grain-boundary processes, such as the formation of point defects, heat capacity, the role of boundaries as sources of vacancies, and internal friction [5, 6]. Incommensurate boundaries were studied by high resolution electron microscopy [7–11] and computer simulation [12, 13]. Boundaries of this type are also widespread in nanocrystalline materials [10, 14]. There is evidence [15] that the presence of incommensurability at the interface between the sample and the film deposited on its surface significantly affects its antioxidant properties. The ideas about relationship between the tribological properties of samples and the structure of surface layers have become widespread. The relationship between microstructure and friction allows not only to estimate the lowest possible coefficient of friction between pure metals and alloys, but also suggests the possibility of creating materials with a low coefficient of friction using grain boundary technology. The connection between the mechanisms of interfacial deformation and friction modes can also be interpreted in an atomistic sense using the concept of commensurate and incommensurable interfaces [16].

An attempt to describe the mechanism of boundary migration was proposed in [17]. Under conditions of boundary displacement along its normal, the introduction of the third component of the discrepancy parameter vector is required. In the general case, it is defined as the radius vector of an atom of one grain in the coordinate system associated with the unit cell of the potential relief of another grain. The presence of an effective thermodynamic migration force means an increased free energy of the atoms of one of the grains compared to the atoms of the neighbouring grain. Relaxation in such a system leads to a shift of the interface towards an energetically favourable position, and the growth of one grain at the expense of another. The model predicts a functional dependence of the migration rate on the effective thermodynamic force of a power form with exponents varying from 1 to 3. Such an effect was repeatedly observed in the experiment [18, 19]. There is currently no general microscopic theory of such a relaxation process as boundary migration. The purpose of this study was the development of the ideas of [17] and development of the model for the migration of an incommensurate intercrystalline slope boundary at the atomic level and a description of self-diffusion processes.

2. Migration model of slope boundary

Let us determine the atomic structure of the unrelaxed slope boundary. For this, consider the geometric picture of the imposition of two identical simple cubic lattices, mutually deployed at a non-special angle. The result of the overlay is shown in Fig. 1. The light and dark nodes denote the projections of the atomic rows of the lattices. For plotting a straight line, which is a trace of the boundary plane, it is necessary to leave nodes of only one colour on different sides. Around each such node located near the boundary, a sphere of radius equal to the interatomic distance is drawn as from the centre. Circles which are sections of these spheres by the plane of the figure are shown in Fig. 1. Any other atom cannot enter them according to in the hard sphere model. The boundary atom located in the centre, can move to the darkened area of the circle, where there are no restrictions from neighbouring circles, if there are vacant positions in this part. By analogy with [17], the interior of the darkened part of the circle is the main region. The coordinate axes x and y, slope axis z normal to them and to the plane of the figure are shown in Fig. a. The slope axis has the symbol [001] in all lattices. The slope boundary separates two crystallites with different lattice orientations, mutually rotated to the arbitrary angle relative to the axis z. Nodes of crystallite *2* are shown as black dots. It is believed that they are all filled with atoms, with the exception of nodes in the main regions. The nodes within each main regions are empty and serve as possible places to be filled with atoms. In this case, the lattice of the second crystallite is completed at the expense of the atoms of the first one, and the entire boundary shifts upwards in Fig. 1.

The presence of an effective migration driving force means that each atom of the first crystallite has an excess of energy W compared to the atoms of the second crystallite. The incorporation of the atom in an empty node in the main region leads to the dissipation of excess of energy. As can be seen from Fig. 1, the presence of empty nodes in the main region in the amount of 0, 1, and 2, indicated by the corresponding numbers, is possible. The size of the main region does not allow placing more nodes in it. If all the main regions are transferred along the boundary and combined with one of the boundaries, then we reach the concept of a reduced region [3, 17]. In the reduced region the position of each empty node can be marked and the density of their distribution can be considered. Incommensurate structures are characterised by uniform geometric distribution of nodes in the reduced main region [1]. Each empty node in the main region can be filled with

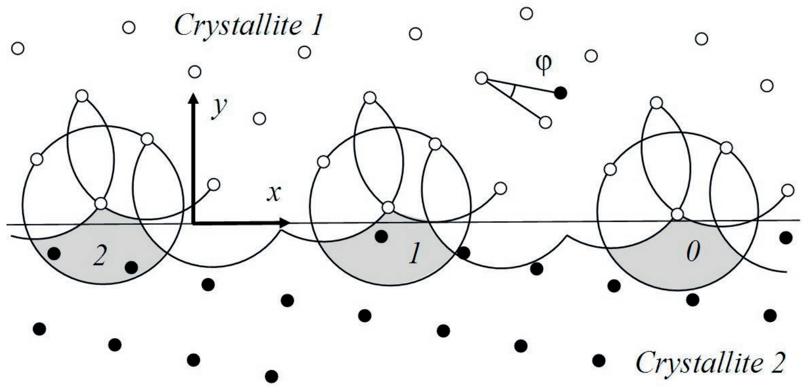


Fig. 1. The picture of the overlapping nodes of the two lattices and the main regions

only one atomic row, its position is unique and serves as the label for this row. Its coordinates are completely similar to the discrepancy parameter introduced earlier for incommensurate structures. The real arrangement of atomic rows due to the relaxation of the structure will differ somewhat from the position of the nodes. However, these nodes determine the most important characteristics of atomic series, such as the activation energy of the transition and the energy in the final arrangement. The thick line in Fig. 2 shows the reduced main region corresponding to the boundary shown in Fig. 1. If one of the nodes of the lattice of the second crystallite falls into the *A* zone, then another node falls into the *A'* zone. The boundaries of the zones are connected by the translation operation for the lattice period of the second crystallite. Only one node can be located in *B* zone. If there are no nodes in the main region, then one of the lattice nodes must necessarily fall into the *C* zone adjacent to the main region. The plotting of the *C* zone is of an auxiliary nature, since its nodes cannot be filled during the migration process. Thus, if the lattice node of the second crystallite falls into one of the zones *A*, *B*, or *C*, then the main region contains 2, 1, or 0 nodes, respectively. Areas of the *A, A′,* and *C* zones equal to each other $S_0 = S_2$. The areas of the *A, B,* and *C* zones are designated as S_2, S_1, and S_0 with an index indicating the number of nodes. The probabilities of the location of nodes in them is $w_i = S_i/S$, where $S = S_0 + S_1 + S_2 = 2S_0 + S_1$ is the total area of the reduced main region.

If the main region contains only one site, then the filling of the vacant row occurs by a thermally activated transition of the atomic row of the first crystallite located at the top of the region, overcoming a barrier equal on average to $W1$. The presence of a barrier is determined by the need to break the bonds of atoms with their immediate neighbours from their crystallite. The transition of the atomic series is a conservative process. It is carried out according to a mechanism similar to a dislocation slip through the formation and propagation of double inflections. The transition time [20] is $\tau_1 = (c_k v_k)^{-1}$, where $c_k = 2a^{-1}\exp(-W_k/kT)$ is the concentration of inflections, v_k is their lateral propagation velocity. This value can be found using the Einstein relation $v_k = D_k F_k/kT$, if we take into account that the force affects the inflection $F_k = Wh/a^2$, and their diffusion coefficient is $D_k = \nu_0 a^2 \exp(-W_{mk}/kT)$. Here W_k and W_{mk} are the energy of formation and migration of the inflection, *h* is its width, equal to the row shift distance, ν_0 is the Debye frequency of vibrations of the atom, *k* is the Boltzmann constant; *T* is the thermodynamic temperature, *W* is the energy difference between atoms in crystallites *1* and *2*. From here it follows that:

$$\tau_1 = \frac{akT}{2\nu_0 Wh}\exp\left(\frac{W_k + W_{mk}}{kT}\right). \tag{1}$$

The inflection energy can be determined [20] from the expression $W_k = 2a\sqrt{2U_P U_0}/\pi$, where $U_P = W_1/a$ is the Peierls energy for a unit length of an atomic series, W_1 is the activation energy of an atom jump to a new position, previously introduced as the barrier value, U_0 is the energy of the unit length of the series. This value can be found by considering the row in the inflection region to be stretched by $\left(l_k{}^2 + h^2\right)^{1/2} - l_k$. Then $W_k = h^2\sqrt{\lambda W_1}/\pi l_k$. Here l_k is the length of the inflection, λ is the stiffness coefficient of the interatomic bond.

In the same way, one of the two nodes that fell into the main region is built up. The second of them is built up by the atoms of the first crystallite from another main region with missing vacant node. This requires the diffusion movement of atoms over a distance between the main regions containing 2 and 0 nodes.

Here we consider the case of sufficiently large values of the migration driving forces. In this case, the process involves all boundary atoms located on one side of the boundary in a layer with a thickness of the order of the lattice period *a*. We call such atomic rows "active". Their number per unit length of the boundary is $N_1 = a^{-1}$. The distribution density of nodes in the reduced area per unit length of the boundary is then equal to $\rho = a^{-3}$. The number of active atomic

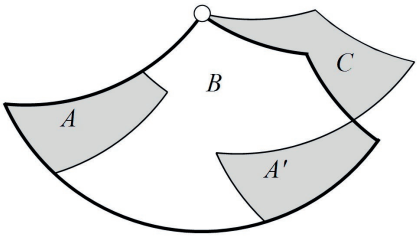


Fig. 2. The reduced main region of the slope boundary

rows with two vacant sites in the main region is $N_2 = \rho w_2 S$. There is the same number of active atomic rows with main regions without nodes. The atoms of the first crystallite from the regions of the last type pass into the main regions with two vacant sites and complete one of them. In the two-dimensional problem, the nodes in the main domain correspond to their rows in the real boundary along *z*. The average distance passed by such atoms along the boundary is:

$$l = \frac{1}{2N_2} = \frac{a^3}{2w_2 S}. \qquad (2)$$

The transition of atoms occurs by diffusion. Transition time:

$$\tau_2 = {}^{l}\!/_{uF}, \qquad (3)$$

where $u = D/kT$ is the mobility of atoms, D is the coefficient of grain boundary diffusion, F is the force required to move atoms from the source to the drain along the boundary. For the driving force of diffusion, we can take the expression $F = W/l$. From formulas (2) and (3), we obtain the transition time:

$$\tau_2 = \left(\frac{a^3}{2w_2 S}\right)^2 \frac{kT}{DW}. \qquad (4)$$

Estimates show that $\tau_2 \gg \tau_1$, therefore the boundary migration rate is limited by diffusion processes in the boundary.

The migrating boundary absorbs vacancies, some of which are redistributed in it and participate in diffusion processes, and some leave the boundary, remaining in a new crystallite. Taking into account that the main regions are densely located at the boundary, it can be assumed that all vacancies are absorbed by only the three types of the described main regions. A vacancy absorbed by an atom that is the centre of the main region of the *A* type, creates three vacant nodes in it. One of them refers to the absorbed atom of the first crystallite, the other two are located at the sites of the second crystallite. It should be noted that before the vacancy was absorbed, there were no vacancies in this region. A vacancy in the boundary is the lattice node in which an atom can be located without the occurrence of a high-energy configuration associated with the displacement of other atoms from their positions. The nodes that were originally available in the main region do not satisfy this condition and therefore are not vacancies. Such a concept of a grain boundary vacancy should be distinguished from an excess volume due to a lattice mismatch in the boundary region. Relaxation in the boundary region leads to the concept of a delocalised vacancy. In the described situation, two vacancies appear in a growing crystallite, since the maximum number of atoms that can be located in it is two. Both of them can fill two nodes of the second crystallite. Filling the vacant position of the first crystallite is associated with energy consumption *W* and restores the atom to its original position, reversing the migration process in the opposite direction, in addition, another atom can no longer be located in this main region. Therefore, we exclude such a process from consideration and take the number of vacancies in this area is equal to two. Using molecular dynamics methods, it was found that the binding energy of vacancies into clusters at the boundary is very low [21], therefore they easily dissociate. This can also be attributed to the two considered vacancies, located in such a way that they form a divacancy in the boundary. One of them can pass into the volume of the second crystallite to replenish their equilibrium concentration in it. The second must be replaced by an atom according to the described scheme. This vacancy leaves its original position and increases the total number of vacancies in the grain boundary system by one.

The absorption of a vacancy of the first crystallite in the main regions with the number of nodes in them equal 1 or 0, by analogy, creates one vacancy or does not create any vacancies. In this case, the appeared vacancy is able to pass into a growing crystallite. Due to the absorption of a vacancy by an atom from the main region of the third described type with a zero number of nodes, the need for its diffusion transition to a vacancy located in the region of the previously considered type with two vacant nodes disappears. The whole described process is equivalent to a simple transition of the atom of the first crystallite from the centre of the main region to one of the sites present in it. Thus, the absorption and emission of vacancies by the boundary does not change the essence of the processes in the main regions and clarifies only the mechanism of transfer of vacancies from one crystallite to another through the boundary.

The total number of vacancies in the boundary participating in diffusion processes is equal to the sum of their equilibrium number in the stationary boundary C_0, vacancies from the main type *A* region and absorbed vacancies in the region without nodes. When the boundary is shifted by a distance *a* it absorbs C_1/a vacancies per unit length, where C_1 is their concentration (atomic fraction) in the first crystallite. They are distributed among the three types of main regions described. Therefore, a region without nodes generates $C_1 w_0/a$ vacancies. Regardless of the absorption of lattice vacancies, each region of the *A* type creates w_2/a vacancies. Therefore, their total concentration in the boundary, taking into account the fact that $w_2 = w_0$, is equal to $C_b = C_0 + w_2\left(1 + C_1\right)$. Neglecting the concentrations in the equilibrium boundary and in the bulk of the crystallite in comparison with w_0, we can assume that <<kul_e029.eps>>.

Based on general principles, we obtain the following expression for the boundary coefficient of self-diffusion:

$$D = \theta a^2 w_2 \nu_0 \exp\left(-\frac{W_m}{kT}\right). \tag{5}$$

Here θ is a geometric factor of the order of unity, W_m is the activation energy of migration of vacancies in the boundary.

3. Discussion

Above, we considered the process of shifting the boundary by a distance *a*. The migration rate is determined by the expression $\upsilon = a\tau^{-1}$. Neglecting the time τ_1 migratory boundary mobility is $I = \upsilon/\sigma$, where $\sigma = Wa^{-3}$ is the value of the effective driving force of migration for a unit area. Using (4), the expression for mobility can be reduced to the form:

$$I = \frac{4Dw_2^2 S^2}{a^2 kT}. \tag{6}$$

When considering the processes of the emergence of vacancies in a migrating boundary, the result, according to which the concentration of vacancies in the boundary is equal to $C_b = w_2$ was obtained. This is a very large value. It can explain the high diffusion mobility of atoms in the migrating boundary [22, 23]. It should be noted that the majority of vacancies in the boundary are not of thermal origin, but are determined only by the geometric atomic structure of the migrating boundary. The expression for the boundary diffusion coefficient now does not contain a factor that depends on the activation energy of vacancy formation. Using such an approach, it is easy to understand the observed increase in the boundary self-diffusion coefficient in migrating boundaries [24–26]. The structural state of grain boundaries during their migration is essentially nonequilibrium [24]. It can be compared with stationary nonequilibrium grain boundaries in freshly prepared ultra-fine-grained materials. As it is known, they contain a significant excess free volume in the form of delocalised vacancies [27]. The diffusion activation energy in such boundaries can be two times lower than in boundaries with an equilibrium structure [28]. The nonequilibrium of migrating boundaries is associated by many authors with an increase in the free volume in the boundary, which is either the result of the absorption of excess vacancies in the volume of the disappearing grain, or the capture of dislocations with their subsequent dissociation [27, 29]. In the present study, the mechanism of generation of vacancies inside the boundary is described without taking into account all these processes. Here, the degree of nonequilibrium of the boundary is determined only by local atomic rearrangements. The effects listed above can have an additional influence, leading to an increase in the degree of nonequilibrium. An increase in the excess volume in the boundary inevitably leads to its broadening.

Let us estimate the ratio of the boundary self-diffusion coefficients in the migrating and stationary boundaries. We accept for the latter the expression $D_e = \lambda a^2 \nu_0 \exp(-(W_f + W_m)/kT)$, where W_f and W_m are the energies of formation and migration of grain boundary vacancies, λ is the coefficient. Taking into account (5), this ratio is $n = D/D_e = w_2 \exp(W_f/kT)$. Here $\theta \approx \lambda$ is accepted. Taking $w_2 \approx 0.1$; $W_f \approx 0.4W_b$, where $W_b = W_f + W_m$ is the activation energy of grain boundary self-diffusion; $W_b/kT_m = 9$ [27]; $T_m/T = 0.5$, T_m is melting temperature; we obtain $n \approx 1.3\cdot 10^2$, which agrees with the experimental data for the migrating boundary $n \sim 10^2$ [24]. In [30], the experimentally measured value of the diffusion coefficient of Ca into calcite at a temperature of 900 °C at the migrating boundary exceeded its value for the stationary boundary by five orders of magnitude. It should be noted that there is a fundamental difference between the nonequilibrium structures in the considered cases of a moving boundary during its migration and a solid boundary in nanostructured systems. When the boundary stops, the nonequilibrium concentration of vacancies in it, after a certain relaxation time, reaches the value characteristic for the stationary boundary. This nonequilibrium is dynamic in nature, when vacancies are continuously generated in the moving boundary and disappear. The non-simultaneity of these processes leads to an excess of vacancies in the boundary. Stationary grain boundaries can be called nonequilibrium if they have an excess free volume, increased energy, or are sources of dislocations [31–34]. The disequilibrium of the boundaries is often associated with the presence of long-range stress fields, while in the migrating boundary, according to the described model, they are absent.

4. Conclusions

Based on the concept of the atomic structure of an incommensurate intercrystalline slope boundary, a model of its migration has been developed. It was shown that the rearrangement of atomic configurations in the boundary region has both local and non-local nature with the involvement of diffusion processes. The relaxation of the atomic structure leads to the fact that the concentration of vacancies in the migrating boundary exceeds that in the stationary boundary. This causes an increase in the self-diffusion coefficient along such a boundary.

Author contributions

V. G. Kul’kov – idea, model development, article writing.

Conflict of interests

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

1. Darinskii B. M., Saiko D. S., Fedorov Yu. A. Sliding along the boundary forming an incommensurable structure*. *Izvestiya vysshikh uchebnykh zavedenii. Fizika = Russian Physics Journal*. 1987;30(9): 53–57. https://www.elibrary.ru/item.asp?id=36961888 (In Russ.)

2. Żydek A., Wermiński M. and Trybula M. Description of grain boundary structure and topology in nanocrystalline aluminum using Voronoi analysis and order parameter. *Computational Materials Science*. 2021;197: 110660. https://doi.org/10.1016/j.commatsci.2021.110660

3. Darinskii B. M., Kul’kov V. G. Intercrystalline sliding along the boundaries formed by densely packed planes*. *Poverkhnost’. Fizika, khimiya, mekhanika = Physics, Chemistry and Mechanics of Surfaces*. 1993;75(5): 153–156. https://www.elibrary.ru/item.asp?id=36705071 (In Russ.)

4. Shtremel M. A., Markovich A. L. Energy of incommensurate grain boundaries. *The Physics of Metals and Metallography*. 1991;71(6): 21–29. https://www.elibrary.ru/item.asp?id=31078891

5. Darinskii B. M., Kalinin Yu. E., Mushtenko S. V., Saiko D. S. Structure of grain boundaries of a general type and mechanism of grain boundary internal friction peak. *Solid State Phenomena*. 2003;89: 203–232. https://doi.org/10.4028/www.scientific.net/SSP.89.203

6. Darinskii B. M., Kalinin Y. E., Sajko D. S. Atomic structure of the intercrystalline general type boundaries. Mechanisms of the grain boundary peak of internal friction. Premelting. *Solid State Phenomena*. 2006;115: 73–86. https://doi.org/10.4028/www.scientific.net/SSP.115.73

7. Gautam A., Radetic T., Lancon F., Dahmen U. Quantitative study of an incommensurate grain boundary using aberration corrected microscopy. *Microscopy and Microanalysis*. 2011;17(S2): 1338–1339. https://doi.org/10.1017/S1431927611007562

8. Gautam A., Ophus C., Lancon F., Radmilovic V., Dahmen U. Atomic structure characterization of an incommensurate grain boundary. *Acta Materialia*. 2013;61(13): 5078–5086. https://doi.org/10.1016/j.actamat.2013.04.028

9. Deymier P. A., Shamsuzzoha M., Weinberg J. D. Experimental evidence for a structural unit model of quasiperiodic grain boundaries in aluminum. *Journal of Materials Research*. 1991;6(7): 1461–1468. DOI: https://doi.org/10.1557/JMR.1991.1461

10. Lancon F., Ye J., Caliste D., Radetic T., Minor A. M., Dahmen U. Superglide at an internal incommensurate boundary. *Nano Letters*. 2010;10(2): 695–700. https://doi.org/10.1021/nl903885p

11. Wang Sh., Yu Yue, Zhang Sh., Zhang Sh., Xu H., Zou X., Zhang J., Atomic-scale studies of overlapping grain boundaries between parallel and quasi-parallel grains in low-symmetry monolayer ReS_2. *Matter*. 2020;3(6): 2108–2123. https://doi.org/10.1016/j.matt.2020.09.015

12. Rouviere J., Lancon F., Rousseau K., Caliste D., Jouneau P., Fourne F. Structure of an incommensurate 90° Si grain boundary resolved with the help of a Cs-corrector for illumination. *Journal of Physics: Conference Series*. 2010;209: 012041. https://doi.org/10.1088/1742-6596/209/1/012041

13. Sutton A. P. An analytic model for grain-boundary expansions and cleavage energies. *Philosophical Magazine A*. 1991;63(4): 793–818. https://

doi.org/10.1080/01418619108213914

14. Farkas D., Froseth A., Swygenhoven H. Grain boundary migration during room temperature deformation of nanocrystalline Ni. *Scripta Materialia*. 2006;55(8): 695–698. https://doi.org/10.1016/j.scriptamat.2006.06.032

15. Wang L., Qi J., Zhang S., Ding M., Wei W., Wang J., Zhang Zh., Qiao R, Zhang Zh., Li Z., Liu K., Fu Yu., Hong H., Liu C., Wu M., Wang W., He Yu., Cu Yi., Li Q., Bai X., Liu K. Abnormal anti-oxidation behavior of hexagonal boron nitride grown on copper. *Nano Research*. 2022. https://doi.org/10.1007/s12274-022-4388-1

16. Chandross M., Argibay N. Friction of metals: A review of microstructural evolution and nanoscale phenomena in shearing contacts. *Tribology Letters*. 2021;69:119. https://doi.org/10.1007/s11249-021-01477-z

17. Kul'kov V. G., Polyakov A. S. Migration of an incommensurate high_angle grain boundary. *Russian Metallurgy (Metally)*. 2012;(4): 263–268. https://doi.org/10.1134/S0036029512040064

18. Gupta B. K., Madhuri M. K., Gupta S. P. Diffusion induced grain boundary migration in the Cu–Cd system. *Acta Materialia*. 2003;51(17): 4991–5000. https://doi.org/10.1016/S1359-6454(03)00325-2

19. Viswanathan R., Bauer C. L. Kinetics of grain boundary migration in copper bicrystals with [001] rotation axes. *Acta Metallurgica*. 1973;21(8): 1099–1109. https://doi.org/10.1016/0001-6160(73)90026-6

20. Hirth J., Lothe J. *Theory of Dislocations*. John Wiley and Sons; 1982. 857 p.

21. Li X., Liu W., Xu Y., Liu C. S., Fang Q. F., Pan B. C., Wang Zh. Energetic and kinetic behaviors of small vacancy clusters near a symmetric Σ5(310)/[001] tilt grain boundary in bcc Fe. *Journal of Nuclear Materials*. 2013;440(1–3): 250–256. https://doi.org/10.1016/j.jnucmat.2013.05.021

22. Smidoda K., Gottschalk W., Gleiter H. Diffusion in migrating interfaces. *Acta Metallurgica*. 1978;26(12): 1833-1836. https://doi.org/10.1016/0001-6160(78)90095-0

23. Krasil'nikov, V. V., Savotchenko, S. E. Grain boundary diffusion patterns under nonequilibrium and migration of grain boundaries in nanoctructure materials. *Bulletin of the Russian Academy of Sciences: Physics*. 2009;73(9): 1277–1283. https://doi.org/10.3103/S1062873809090214

24. Gorelik S. S, Dobatkin S. V., Kaputkina L. M. *Recrystallization of metals and alloys**. M.: MISIS Publ.; 2005, 432 p. (In Russ.)

25. Prokoshkina D., Klinger L., Moros A., Wilde G., Rabkin E., Divinski S.V. Effect of recrystallization on diffusion in ultrafine-grained Ni. *Acta Materialia*. 2014;69: 314–325. https://doi.org/10.1016/j.actamat.2014.02.002

26. Chuvil'deev V. N., Nokhrin A. V., Pirozhnikova O. E., Gryaznov M. Y., Lopatin Y. G., Kopylov V. I., Myshlyaev M. M. Changes in the diffusion properties of nonequilibrium grain boundaries upon recrystallization and superplastic deformation of submicrocrystalline metals and alloys. *Physics of the Solid State*. 2017;59(8): 1584–1593. https://doi.org/10.1134/S1063783417080066

27. Chuvil'deev V. N. *Nonequilibrium grain boundaries in metals. Theory and applications**. M.: Fizmatlit Publ., 2004. 304 p. (In Russ.)

28. Kim H. K. Activation energies for the grain growth of an AZ31 Mg alloy after equal channel angular pressing. *Journal of Materials Science*. 2004;39(23): 7107–7109. https://doi.org/10.1023/B:JMSC.0000047560. 93940.45

29. *Physical Metallurgy*. Edited by R. W. Cahn, P. Haasen, North-Holland Physics Publishing, 1983, 1973 p.

30. McCaig A., Covey-Crump S. J., Ben Ismaïl W., Lloyd. G. Fast diffusion along mobile grain boundaries in calcite. *Contributions to Mineralogy and Petrology*. 2007;153: 159–175. https://doi.org/10.1007/s00410-006-0138-8

31. Tucker G. J., McDowell D. L. Non-equilibrium grain boundary structure and inelastic deformation using atomistic simulations. *International Journal of Plasticity*. 2011;27(6): 841–857. https://doi.org/10.1016/j.ijplas.2010.09.011

32. Nazarov A. A., Murzaev R. T. Nonequilibrium grain boundaries and their relaxation under oscillating stresses in columnar nickel nanocrystals studied by molecular dynamics. *Computational Materials Science*. 2018;151: 204–213. https://doi.org/10.1016/j.commatsci.2018.05.015

33. Wang Yu., Fu R., Jing L., Sang D., Li Yi. Tensile behaviors of pure copper with different fraction of nonequilibrium grain boundaries. *Materials Science and Engineering: A*. 2018;724: 164–170. https://doi.org/10.1016/j.msea.2018.03.086

34. Chuvil'deev V. N., Kopylov V. I., Zeiger W. A theory of non-equilibrium grain boundaries and its applications to nano- and micro-crystalline materials processed by ECAP. *Annales de Chimie Science des Materiaux*. 2002;27(3): 55–64. https://doi.org/10.1016/S0151-9107(02)80007-1

*Translated by author of the article.

Information about the author

Viktor G. Kul'kov, Dr. Sci. (Phys.–Math.), Associate Professor, Professor at the Volzhsky Branch of National Research University «Moscow Power Engineering Institute» (Volzhsky, Russian Federation).

https://orcid.org/0000-0001-8449-026X

vikulkov@yandex.ru

Received 13.06.2022; approved after reviewing 18.07.2022; accepted for publication 15.09.2022; published online 25.12.2022.

Translated by Valentina Mittova
Edited and proofread by Simon Cox