Studying Grain-Boundary Stresses in Copper by the Molecular-Statics Method

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Abstract—Grain-boundary stresses in copper for 60 symmetrical tilt grain boundaries with different orientations of the grain-boundary plane and tilt axis have been calculated by the molecular-statics method with the use of embedded-atom-method potentials of interatomic interaction. It has been established that the grain-boundary stresses are negative for grain boundaries with small excess volumes and increase approximately linearly with a buildup of the excess volume. It has been shown that the increase in grain-boundary stresses is connected with a decrease in the average coordination number of atoms, whereas pairs of closely spaced atoms in the grain-boundary core cause a negative contribution to grain-boundary stresses.

INTRODUCTION

The grain-boundary (G-B) stresses described by a second-rank tensor serve as macroscopical characteristics of grain boundaries and represent a particular case of interface stresses at interphase boundaries where at least one of the adjacent phases is a solid. Although a thermodynamic definition of interface stresses (ISs) was first given by Gibbs at the beginning of the past century, these stresses and their effect on the properties of interphase boundaries have been actively investigated only in the last two decades, predominantly for the case of surface stresses (stresses at an interphase boundary between solid and gaseous phases). Unlike the surface tension, which is numerically equal to the surface energy required for the work on creating a new surface to be done, the surface stresses are determined by the work necessary for elastic deformation of the interphase boundary in a reversible manner [1, 2].

At present, there are numerous examples of the determining role of ISs in the development of diffusional processes and in the formation of the structure and physical properties of interphase boundaries. In particular, such examples are considered in the reviews by Ibach [1] and Spaepen [2]. For instance, G-B stresses play a large role in the process of grain-boundary diffusion and related phenomena [3], which is of prime importance for nanostructured materials [4, 5], in which the atoms in grain boundaries constitute a good fraction of the total number of atoms. A systematic study of G-B stresses is now in progress [2, 6]. Recently, several works devoted to the experimental determination of averaged values of G-B stresses in metals (see [6] and references therein) were published. The measured average value of G-B stresses in palladium was found to be 1.2 J/m^2, which is half as high again as typical values of the surface tension for high-angle grain boundaries in Pd (0.8 J/m^2) [6]. In other words, the G-B stress differs substantially from the G-B tension and is an important thermodynamic characteristic of grain boundaries (GBs). On the other hand, we know only one theoretical calculation of G-B stresses performed for the $\Sigma 3(112)$ grain boundary in aluminum in the context of analyzing the phenomenon of faceting [7].

Being macroscopic characteristics, the G-B stresses, on the other hand, are associated with an atomic structure and features of interatomic interaction in the GB core. In this connection, it is of interest to establish interrelations between G-B stresses and characteristics of the atomic structure of GBs. It is convenient to choose the excess volume as a generalized characteristic of GBs on the atomic scale. The excess volume is of great importance for the description of properties of grain boundaries. Calculations of the excess volume in fcc and bcc metals showed that this quantity is directly connected with the G-B energy [8]. The G-B energy increases approximately linearly with a buildup of the excess volume [8]. Besides, a correlation is traced between the excess volume and a number of fundamentally important properties of grain boundaries: G-B segregation, corrosion along GBs, migration of GBs in the process of recrystallization, etc. [8]. In this connection, revealing dependences between the G-B stresses and the excess volume can be of considerable importance in solving the problem of establishing a relation between the properties of grain boundaries and their thermodynamic characteristics.

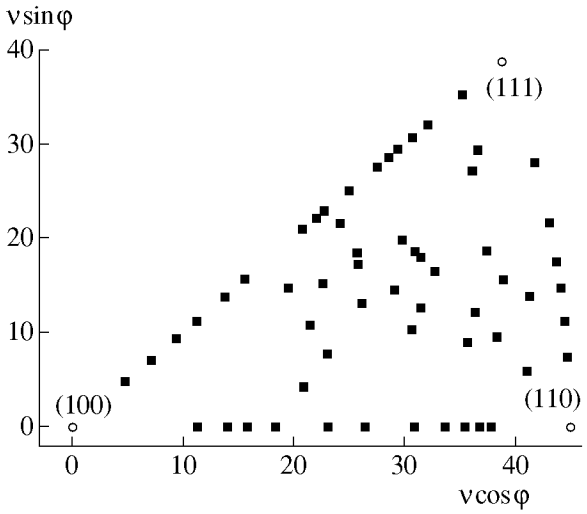

Fig. 1. Position of symmetrical tilt grain boundaries (black squares) considered in this work; ν and φ are the polar and the asimuthal angles characterizing the direction of the normal [*hkl*] to the GB plane.

It is natural to study the dependence between the G-B stresses and the atomic structure of GBs by computer simulation on the atomic scale, when the coordinates of all the atoms are specified. In this work, such an investigation on the example of high-angle symmetrical tilt GBs in copper at 0 K was performed by the molecular-statics method using the embedded-atom method (EAM) [9]. At present, this method virtually became a standard for the specification of model potentials of interatomic interactions in metals and, in particular, passed an evaluation test when studying the defect structure of surfaces of fcc metals with low [10] and high [11] Miller indices and also when investigating the mechanism of grain-boundary diffusion in copper [12]. In this work, we established the main tendencies in the changes in the G-B stresses with varying excess volume and explained them proceeding from the general properties of the atomic structure of GBs in metals.

QUALITATIVE DESCRIPTION OF GRAIN-BOUNDARY STRESSES

A GB is a planar crystal-structure defect. In the GB core, the equilibrium bond lengths between atoms differ from those in the perfect lattice. However, the atomic GB structure does not reach a complete relaxation because of limitations related to the effect of adjacent grains. For this reason, in a system with GBs, stresses are present even in the case where all the atoms occupy positions corresponding to the minimum of free energy of the system. The two-dimensional tensor of grain-boundary stresses can be defined analogously to the ordinary three-dimensional tensor of stresses in the theory of elasticity.

Let us consider a fragment of a polycrystal with one GB having an area A and a G-B energy per unit area γ. Upon elastic deformation of the fragment, a work against G-B stresses is done in the G-B plane, which increases the G-B energy:

$$A\sum_{\alpha\beta}\tau_{\alpha\beta}d\varepsilon_{\alpha\beta} = d(A\gamma) = \sum_{\alpha\beta}\frac{\partial(A\gamma)}{\partial\varepsilon_{\alpha\beta}}d\varepsilon_{\alpha\beta}. \qquad (1)$$

In view of the arbitrariness of small deformations $d\varepsilon_{\alpha\beta}$, we obtain from Eq. (1) the following expression for the components of the tensor of G-B stresses:

$$\tau_{\alpha\beta} = \frac{1}{A}\frac{\partial(A\gamma)}{\partial\varepsilon_{\alpha\beta}} = \gamma\delta_{\alpha\beta} + \frac{\partial\gamma}{\partial\varepsilon_{\alpha\beta}}, \qquad (2)$$

where $\delta_{\alpha\beta}$ are the Kronecker δ symbols, and the partial derivatives are taken with respect to components $\varepsilon_{\alpha\beta}$ of the deformation tensor in the G-B plane. This is the well-known equation that describes stresses (not only G-B stresses) at interphase boundaries. Although it is also possible to introduce other equivalent definitions of the tensor $\tau_{\alpha\beta}$ (see the recent review [1]), Eq. (2) is convenient for discussing the sign of $\tau_{\alpha\beta}$ and obtaining calculation formulas. If the sign of γ is always positive (the formation of GBs increases the free energy of the system), there are no restrictions on the sign of the derivative $\partial\gamma/\partial\varepsilon_{\alpha\beta}$ (and on the sign of G-B stresses). The quantity $\tau = \sum\tau_{\alpha\alpha}/2$ (an analog of the pressure $P = \sum\sigma_{ii}/3$ for the three-dimensional tensor of elastic stresses σ_{ij}) is a scalar characteristic of G-B stresses. In the case of tensile stresses in a GB (the GB tends to decrease its area), the G-B stress τ is taken to be positive.

GEOMETRY AND METHOD OF CALCULATION

The unrelaxed structures of symmetrical tilt grain boundaries (STGBs) considered in this work were constructed by rotating one half of an ideal fcc crystal through 180° about the normal to the grain-boundary plane (*hkl*). Such a construction is justified, since all STGBs can be considered as twins with an inverse interchange of the sequence of packing of atomic planes upon the passage through the boundary plane [13]. For the structures thus constructed, the procedure of relaxation was performed by the molecular-dynamics (MD) method with damping of atomic velocities. The damping consisted in zeroing of the velocity of an atom at each step of the MD procedure if the scalar product of the vectors of the velocity and the force acting on the atom was smaller than zero. In order to minimize the G-B energy with respect to G-B displacements, we specified the relative displacements of grains in the G-B plane prior to the performance of the relaxation procedure, and the relaxation involved G-B displacements. In doing so, a uniform two-dimensional

grid of initial G-B displacements including from 100 to 400 nodes depending on the unit-cell size in the G-B plane was employed. The high-angle STGBs considered in this work are shown in Fig. 1, in which the orientations of the GBs are given according to the graphic construction suggested by Wolf [13]. As is seen from Fig. 1, the GBs considered are approximately uniformly distributed over the entire region of high-angle STGBs in an fcc crystal. The realized sample of orientations contained 60 GBs in copper with the reciprocal density of coincident sites from $\Sigma = 3$ to $\Sigma = 253$.

In this work, we used the well-known model that fairly well describes GBs in a bicrystal [14]. In this model, the G-B structure is periodic in the x and y directions belonging to the boundary plane, but is limited on both sides by rigid atomic layers in the z direction perpendicular to the boundary plane. The thickness of each rigid layer was not less than two radii of interatomic interaction r_c, which excluded the effect of an artificial cutoff of the bicrystal in the directions perpendicular to the G-B plane. The thickness of each grain in the region between rigid layers was not smaller than $3r_c$ per grain, and the doubling of this thickness changed the values of calculated G-B stresses varied no more than by 10^{-4} J/m^2. Although the atoms of the rigid layers were fixed in the sites of the ideal lattice, the layers during relaxation were displaced under the action of forces from the other atoms of the model, thereby ensuring the possibility of the relative displacement of grains of the model bicrystal. There were no restrictions on the atomic displacements between the layers. As the criterion for the exit from the procedure of relaxation, we assumed the simultaneous fulfillment of two conditions given below. First, forces acting on the atoms located between the rigid layers should not be more than 0.001 eV/Å. Second, the total forces per unit GB area acting on each rigid layer must not exceed 10^{-6} GPa.

To specify the interatomic interaction in copper, we employed the EAM potentials constructed by Mishin *et al.* [15] and the results of first-principles calculations of energies of model systems of copper. These potentials satisfactorily reproduce the sublimation energy, elastic constants, energy of formation and migration of vacancies, and energy of formation of stacking faults; recently, they were applied to study the mechanisms of G-B diffusion in copper [12]. In the embedded-atom method [9], the configurational energy E of the atomic system can be represented as the sum of contributions E_i from atoms i:

$$E = \sum_i E_i = \sum_i \left\{ F_i[\bar{\rho}_i] + \frac{1}{2}\sum_j \Phi_{ij}(R_{ij}) \right\}, \qquad (3)$$

where $\bar{\rho}_i = \sum_{j\neq i} \rho_j(R_{ji})$ is the superposition of atomic densities $\rho_j(R_{ji})$ at the location of atom i, which is created by all the remaining atoms of the system; $F[\rho]$ is the function of embedment; and $\Phi(R)$ is the pair potential as a function of the interatomic distance R.

Ackland and Finnis [16] obtained an expression for the components of the tensor of surface stresses in the framework of the EAM (see also [17]). For this reason, we give an analogous expression for the components of the tensor of G-B stresses without discussion of the details of its derivation. Assuming that body stresses disappear as the distance from a GB increases, the tensor of G-B stresses is described by the expression

$$\tau_{\alpha\beta} = \frac{1}{A}\sum_i \sum_{j(>i)} \left(F_i'[\bar{\rho}_i]\frac{\partial \rho_j(R_{ji})}{\partial R_{ji}} + \frac{1}{2}\frac{\partial \Phi_{ji}(R_{ji})}{\partial R_{ji}} \right) \times \frac{R_{ji\alpha}R_{ji\beta}}{R_{ji}} = \sum_i \tau_{\alpha\beta}(i). \qquad (4)$$

Here, $\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i$ is the vector directed from site i to site j, and prime stands for the first derivative of the function of embedment with respect to the argument. Formula (4) determines the components of the tensor of grain-boundary stresses as a sum of contributions $\tau_{\alpha\beta}(i)$ associated with an atom i. Since the stresses are taken to be absent in the bulk of grains, we have $\tau_{\alpha\beta}(i) = 0$ when the atom i is at a sufficiently far distance from the G-B core. This allowed us to calculate $\tau_{\alpha\beta}$ by formula (4) in the framework of the above-described model of the bicrystal by summation over indices i for atoms located between the rigid layers. The other form of representation of the components of the tensor of G-B stresses

$$\tau_{\alpha\beta} = \frac{1}{A}\sum_i \sum_{j(>i)} \left(F_i'[\bar{\rho}_i]\frac{\partial \rho_j(R_{ji})}{\partial R_{ji}} + F_j'[\bar{\rho}_j]\frac{\partial \rho_i(R_{ji})}{\partial R_{ji}} + \frac{\partial \Phi_{ji}(R_{ji})}{\partial R_{ji}} \right)\frac{R_{ji\alpha}R_{ji\beta}}{R_{ji}} = \sum_i \sum_{j(>i)} \tau_{\alpha\beta}(i, j) \qquad (5)$$

determines $\tau_{\alpha\beta}$ as the sum of contributions of atomic pairs. Hereafter, we use this expression to analyze the relation between the G-B stresses and the features of the atomic structure of GBs in metals.

The excess volume defined as an increase in the volume of the system (due to the formation of a GB) per unit G-B area is equal to the relative displacement of grains in the direction perpendicular to the G-B plane. Therefore, the excess volume δV related to a GB is equal, according to the employed model of the bicrystal, to the relative displacement of rigid layers in the z direction as a result of relaxation. The grain-boundary energy γ was calculated by the formula $\gamma = \Sigma(E_i - E_0)/A$, where summing is performed over atoms i of the computational cell between rigid layers, E_i is the contribution of these atoms to the configurational energy,

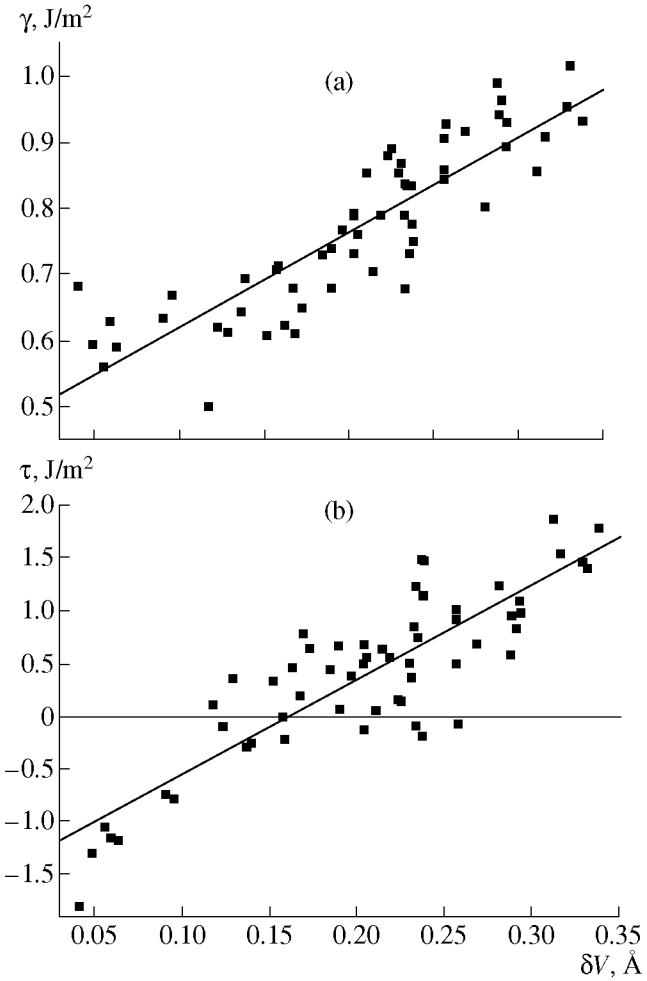

Fig. 2. Dependences of the calculated values of (a) grain boundary energies γ and (b) grain-boundary stresses τ on the excess volume δV. The straight lines in this and subsequent figures are drawn on the basis of a linear interpolation by the least-squares method.

and E_0 is the energy per atom in the ideal lattice. In the embedded-atom method, this expression for the energy γ is exact, since in this method the total energy of the system can be represented as the sum of contributions of individual atoms (see Eq. (3)) and, for the atoms located far from the region of the G-B core, E_i is equal to E_0.

Note here that upon the calculation of the energy γ, the presumed disappearance of stresses in the bulk of grains, which underlie expressions (4) and (5), and the assumption that $E_i = E_0$ far from a GB are not fulfilled strictly because of the finite thickness of the region between the rigid layers. For this reason, we also estimated the scalar stress τ with the use of expression (2), for which purpose the derivatives $\partial\gamma/\partial\varepsilon_{xx}$ and $\partial\gamma/\partial\varepsilon_{yy}$ were calculated numerically by specifying small deformations $\varepsilon_{xx}(\varepsilon_{yy}) = \pm 0.001$ (the effect of the magnitude of deformation was controlled by calculating the derivatives for values 0.01 and 0.0001). Since the accuracy of the calculation of stresses and energy of GBs depends also on the boundary conditions of the problem and the degree of relaxation of the system, the coincidence of the analytically and numerically calculated values of τ, along with the convergence of τ and γ with increasing computational-cell thickness, served as an additional test of the validity of the method.

RESULTS OF CALCULATIONS AND DISCUSSION

Figure 2 displays the results of calculations of the G-B energy γ and the scalar characteristic of G-B stresses τ as functions of the excess volume. As is seen from Fig. 2a, the G-B energy is an approximately linear function of the excess volume, which is in qualitative agreement with the results of calculations of other authors [8]. The proportionality factor determined from the slope of the $\gamma(\delta V)$ straight line is equal to 1.43 (J/m²)/Å with an error of 7.6%. The $\tau(\delta V)$ dependence that was established for GBs in copper likewise is approximately linear, and the corresponding proportionality factor determined with an error of 7.9% is equal to 8.98 (J/m²)/Å (Fig. 2b). It follows herefrom that for GBs with large excess volumes, the τ values are more than half as large again as the γ values. As is seen from Fig. 2b, the grain boundaries with small excess volumes are characterized by negative G-B stresses. Therein lies a fundamental distinction of G-B stresses from G-B tensions, which are determined by the G-B energy and have only positive values. The $\tau(\delta V)$ dependence shown in Fig. 2b has a negative final value in the limit of $\delta V \geq 0$. For this reason, this dependence can be valid only for high-angle grain boundaries.

In order to explain the tendencies in changes in the G-B stresses which we found, we consider the general properties of the atomic structure of high-angle grain boundaries in metals. As a result of numerous theoretical and experimental investigations of grain boundaries on the atomic scale (see the review [8]), it was established that the average density of atoms in GBs is smaller than that in the bulk of crystal (the excess volume of GBs is positive). At the same time, in the GB core there are pairs of atoms the distances between which are smaller than the interatomic distances in the ideal lattice. In spite of a relatively small number of such pairs, they give a significant contribution to the G-B energy. This is caused by the asymmetry of interatomic interactions; the potential energy increases markedly faster when the interatomic distances deviate from the equilibrium bond lengths in the direction of decreasing values than upon their deviation in the direction of increasing values.

To quantitatively describe the atomic structure of GBs, we investigated in this work, along with the

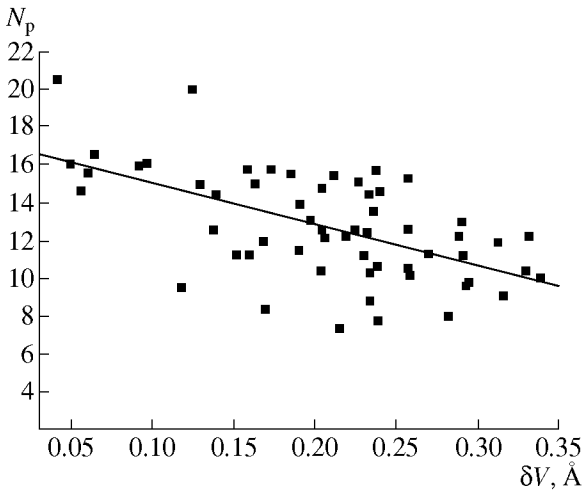

Fig. 3. The calculated numbers N_p of pairs of closely spaced atoms in GBs (see the main text) depending on the excess volume.

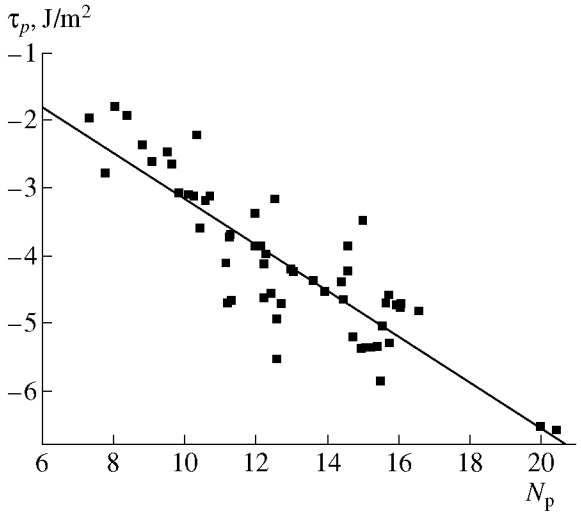

Fig. 4. Calculated contributions τ_p of pairs of closely spaced atoms to grain-boundary stresses τ as a function of the number of pairs N_p.

known qualitative properties of the atomic structure of GBs, the behavior of the quantity

$$N_p = \frac{a_0^2}{A}\sum_m \left[1 - \frac{|\mathbf{n}\mathbf{d}_m|}{|\mathbf{d}_m|}\right], \qquad (6)$$

where summing is performed over pairs of atoms m distances between which are smaller than 98% of the radius of the first coordination shell in the fcc lattice of copper with the equilibrium lattice parameter a_0, $\mathbf{n}$ is the vector of the normal to the G-B plane, $\mathbf{d}_m$ is the vector connecting the sites of atoms in a pair, and A is the G-B area. This quantity characterizes the number of pairs of closely spaced atoms with allowance for the orientation of the pairs with respect to the G-B plane. A pair makes a maximum contribution to N_p when being oriented in parallel with the G-B plane, and the contribution of a pair is equal to zero if it is orientated perpendicularly to the GB. Therefore, it may be expected that the introduced characteristic of the atomic structure of GBs will be related to grain-boundary stresses.

The results of our calculations of the quantity N_p are shown in Fig. 3, which graphically demonstrates the relation between the atomic G-B structure and the excess volume. The GB tends to decrease the excess volume (which is associated with the G-B energy), but this decrease is accompanied by an increase in the number of pairs of closely spaced atoms with a preferred orientation of the pair in the GB plane.

Based on the above-considered features of the atomic structure of GBs in metals, we explain the increase in G-B stresses (Fig. 2) from negative values to values exceeding grain-boundary energies by the action of two factors.

On the one hand, a decrease in the average density of atoms and, hence, a decrease in the average coordination number in the G-B core leads to a shortening of the average equilibrium bond length in GBs with respect to equilibrium bond length in the bulk of grains. This characteristic feature of interatomic interaction in metals—the shortening of the average equilibrium bond with a decrease in the coordination number (a consequence of the retained order of bond [13])—is taken into account in the EAM approximation [13]. However, the average equilibrium bond length in GBs is not achieved because of the restrictions on the local atomic displacement imposed by the interaction with atoms of the adjacent grains. As a result, tensile (positive) stresses are generated in GBs and grow in magnitude with increasing excess volume (with decreasing average density of atoms in GBs).

On the other hand, the closely spaced atoms tend to increase distances between themselves. For this reason, pairs of such atoms make a negative contribution to the magnitude of G-B stresses, and this contribution determines the sign of grain-boundary stresses with small excess volumes. It is essential in this case that the nearer the orientation of a contracted bond to the G-B plane, the more significant is its effect on the G-B stress. This is well seen from Fig. 4, which displays the results of our calculations of contributions to G-B stresses from pairs of atoms (the calculation was performed using expression (5)) distances between which do not exceed 98% of the equilibrium bond length in the fcc lattice of copper. For all the GBs considered, these contributions are negative and grow in absolute value with increasing the above-introduced characteristic of the atomic grain-boundary structure N_p. It also follows from a comparison of Fig. 4 with Fig. 3 that this contribution is most substantial for GBs with small

excess volumes, which accounts for the negative values of G-B stresses at such GBs.

CONCLUSIONS

The dependence of the energies of, and stresses in, 60 high-angle symmetrical tilt grain boundaries in copper with different atomic structures on the magnitude of the excess volume has been investigated on the atomic scale by the method of computer simulation. The results of the studies show an approximately linear increase in the scalar characteristics of G-B stresses with increasing excess volume of GBs which is analogous to the well-known linear dependence for the GB energy [8]. However, the grain-boundary stresses, as distinct from the GB energy, have the negative sign in GBs with small excess volumes and their values in grain boundaries with large excess volumes exceed GB energies by more than a factor of one and a half. The presence of negative G-B stresses and the buildup of G-B stresses with increasing excess volume are explained by the opposite action of two factors: a decrease in the density of atoms and the simultaneous presence in the GBs of interatomic distances that are smaller than the equilibrium lengths of interatomic bonds in the ideal lattice.

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