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Dislocation structure of dicotyledonous bimetals under external harmonic influence: molecular dynamics modeling

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Abstract. In this article, we study the structure of the network of dislocations near the boundary of a dicotyledonous bimetal Ni-Al under intense external harmonic influence. The method of molecular dynamics was chosen as the method, using potentials obtained by the immersed atom method. The paper analyzes the behavior of dislocation segments as a function of the intensity of exposure in the presence of vacancies near the boundary of a bipartite bimetal. It is shown that the frequency of exposure significantly affects the change in the structure of bimetal. In this case, point defects in the form of vacancies play an important role. The analysis was carried out by heating the calculated cells, the temperature of which is not more than half the melting temperature of the materials. Comparison with annealing of defects showed that structural changes in dislocations occur at lower temperatures, and their flow rate is higher.

1. Introduction

With the transition to nanoscale materials, theoretical and experimental interest in bimetallic nanoparticles has sharply increased. The unique physical and chemical properties of bimetallic particles are associated with their structural, electronic, and optical properties [1]. The structure of bimetallic nanoparticles is determined by the distribution of metals in it. Particles can be organized as an ordered alloy, for example, dicotyledonous bimetals, have an arbitrary composition, or have a core-shell architecture. Such materials attract considerable research interest in connection with their potential application in the field of heterogeneous catalysis, since they are often more active in comparison with their monometallic analogues. The improvement in the properties of these systems is associated with the complex interaction of the electrons of two metals and the effects of changes in the lattice parameters in bimetallic alloys or at the interfaces between the two metals [2, 3].

Of particular interest are the Ni-Al compound. Bimetallic nanoclusters are of practical importance for the formation of current and potential contacts in electronics due to the fact that the electron work function strongly depends on the real structure of bimetals. In addition, thin Ni – Al coatings are actively used for reactive chemical bonding of semiconductor structures into multilayer integrated circuits in order to increase the packing density of individual elements due to the implementation of three-dimensional architecture [4–6].



In interpreting many of the physicomachanical properties of real crystals, an important role is played by defects in the crystal lattice, especially dislocations. The mobility of dislocations determines such important mechanical properties of a crystal as ductility and strength. The movement of dislocations under the action of external periodic influences occurs in nonlinear potential fields of internal stresses, which can be caused by various reasons, among which is the periodic relief of the crystal lattice itself and/or other defects of the crystal lattice of various types, in particular, point, linear, etc. External periodic effects can be constant or variable over time. By their nature, variable external influences are very diverse both in origin and in nature, shape and frequency of change. Variable external influences excite forced oscillations of a dislocation of various amplitudes. In the case of a small oscillation amplitude, the linear force law of interaction is a good approximation. If the amplitude of the forced oscillations is sufficiently large, the force law of interaction in the system may already be a nonlinear function of the position of the dislocation.

The influence of periodic external influences on the dislocation and the related possibilities of studying the dynamic properties and internal microstructure of crystals have been studied in sufficient detail [7–12]. Nevertheless, harmonic external influences do not exhaust the entire possible spectrum of external influences on the material. In a number of practically important cases, the dislocation structure of the crystal is exposed to precisely random forces (radiation exposure, vibrations of various thermomechanical nature). For example, in the process of radiation exposure to a crystal, a random flow of elastic impulses to a dislocation can form in it. Random flows form a time-varying force acting on the dislocation. The response of the system to the influence of random forces will depend both on the properties of the system and on the statistical characteristics of the resulting force, including its correlation function. If the random force is a delta-correlated random process of the Gaussian type, then its effect on the mechanical system can be described within the framework of the approximation of the Einstein – Fokker equation [15, 16]. The situation changes if the delta-correlation property is violated. In this case, the Einstein-Fokker approximation is incorrect, the behavior of the system substantially depends on the correlation properties of a random external influence. This circumstance allows us to use the dislocation energy absorption of random acoustic waves as an additional source of information on the dislocation structure of the crystal.

The effect of constant external influences on the crystal dislocation system can also lead to nontrivial dynamic behavior [13, 14]. A typical example is the movement of a dislocation segment in the Peierls-Nabarro relief. Movements of this type are essentially nonlinear, which makes it extremely difficult to analyze. An experimental study of nonlinear dynamic effects during the movement of dislocations is currently complicated by the insufficient theoretical study of this topic. Therefore, an important task is the development of methods for the theoretical description of nonlinear oscillations in problems of the dynamics of dislocations. This determines the relevance of a theoretical study of the dynamic behavior of dislocation systems under the influence of random external influences of various types and the development of theoretical approaches to the study of the essentially nonlinear dynamic behavior of such systems.

If the external action is a random process, then the displacement of the dislocation, determined by the solution of the equation of oscillations, is also a random process. In the linear case, by representing the solution in the form of a Fourier series, it is possible to show that the damping decrement is determined by the correlation function of the external voltage. The nonlinear case is much more complicated. Analytically, one can figure it out only by neglecting inertial effects and considering spatially uniform dislocation motions. But even in this case, one can find the dependence of the behavior of the dislocation on the correlation properties of the external action [15]. Attempts to take into account the inertial properties of a dislocation oscillating in a nonlinear potential relief were unsuccessful due to the impossibility of using analytical methods. Moreover, the problem of describing the nonlinear motion of a dislocation is far from its solution even in the case of periodic external influence.

A number of our studies [16–19] studied the behavior of this bimetal under intense external influences in the form of shock waves. Some dynamic effects and structural changes in crystals are considered.

Here we consider the effect of the external periodic influence at the frequencies of the phonon spectra of crystals of Ni-Al bimetal on the dislocation network of the boundary of dicotyledonous bimetals in the presence of point defects in the form of vacancies. What can be useful in constructing a theory of the motion of dislocations in nonequilibrium systems.

2. Research methods

The processes studied in the work are distinguished by a high flow rate, which makes direct observation difficult. Therefore, the most optimal is the use of computer simulation methods. The method of molecular dynamics was chosen as the method of molecular dynamics, due to the fact that it allows you to conduct experiments with given atomic velocities and describe the dynamics of the processes under study in real time. This method has proven itself in the study of processes at the interface between metals and alloys [20]. The study was conducted using the LAMMPS Molecular Dynamics Simulator package [21], which has an extensive set of supported potentials. For calculations, the nvidia tesla k40 graphics accelerator was used, which allows performing calculations with double precision.

As a potential function of interatomic interaction, we used the potential included in the standard LAMMPS set calculated using the immersed atom method. The total energy of the crystal E in this case can be expressed as:

$$E = \frac{1}{2} \sum_{i,j,i \neq j} \varphi_{ij}(r_{ij}) + \sum_i F_i(\rho_i), \quad (1)$$

where φ_{ij} represents the pair energy between atoms i and j , separated by a distance r_{ij} , and F_i – embedding energy associated with an embedded atom i in a local location with electron density ρ_i . The electron density can be calculated by the formula:

$$\rho_i = \sum_{j,j \neq i} f_j(r_{ij}), \quad (2)$$

where $f_j(r_{ij})$ – electron density at the site of atom i located at a distance r_{ij} from the atom j .

The temperature of the computational cell was set by assigning random speeds to the atoms in accordance with the Maxwell-Boltzmann distribution. The step of numerical integration of the equations of motion was 1 fs.

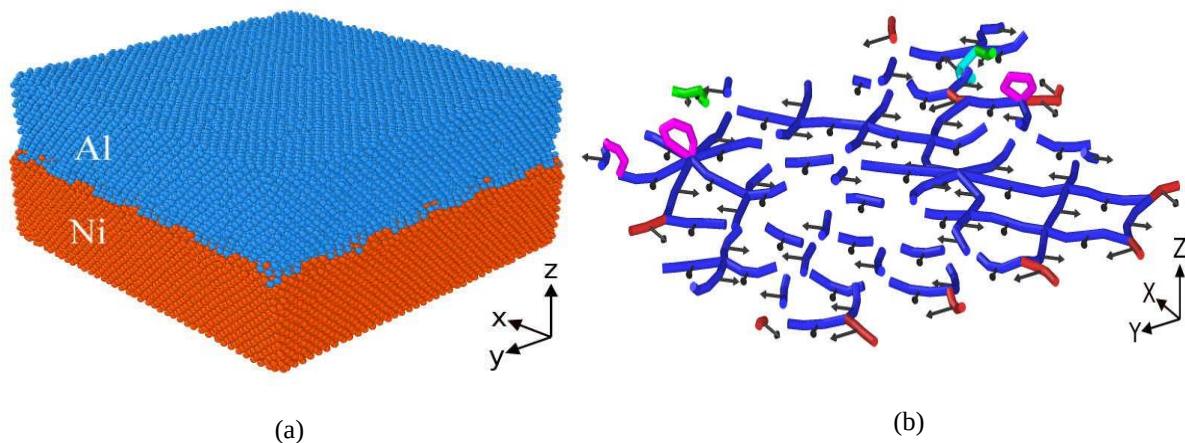


Figure 1. Dicotyledonous bimetal model: (a) Three-dimensional view of a Ni-Al particle containing $4.5 \cdot 10^5$ atoms; (b) a network of dislocations at the boundary of metals with the indication of Burgers vectors (blue – perfect dislocation, violet – Strain-rod dislocation, green – Shockley dislocation, light blue – Frank dislocation, red – other dislocation).

The model of a dicotyledonous bimetal (figure 1 (a)), which has the shape of a rectangular parallelepiped, was considered in the work; the number of atoms in the computational cell was $4.5 \times$

105. To obtain dicotyledonous model bimetals, two initial single-component crystals of different metals were placed at a distance of about 2.5 Å from each other. After that, the structure was relaxed under free boundary conditions along all axes. Then 3% of atoms were removed randomly in bimetal, thereby forming vacancies. Repeated relaxation was performed with cooling of the model to 5 K.

After repeated relaxation, a characteristic network of dislocations was formed at the metal boundary (figure 1 (b)). Periodic harmonic effect was carried out by law $Z = A \sin(\omega t)$, where A – amplitude of external influence, ω – region oscillation frequency. These harmonic laws were introduced through commands of mathematical functions built into LAMMPS and variables. Oscillations were carried out along the Z axis with frequencies from 0.1 to 0.2 THz, and with amplitudes from 0.05 Å. This range allows us to cover part of the spectrum of low-amplitude atomic vibrations for the bimetal under consideration. At least three computer experiments with the same initial parameters were performed to compare the results.

3. Results and discussions

At the initial stage, the change in the dislocation structure upon heating of a dicotyledonous bimetal was studied. The time dependence of the length of dislocation segments was considered (figure 2 (a)) by type of dislocation. In this case, the total length of the dislocation network remained approximately the same. Vacancies were concentrated mainly at the nodes of the network of misfit dislocations after relaxation.

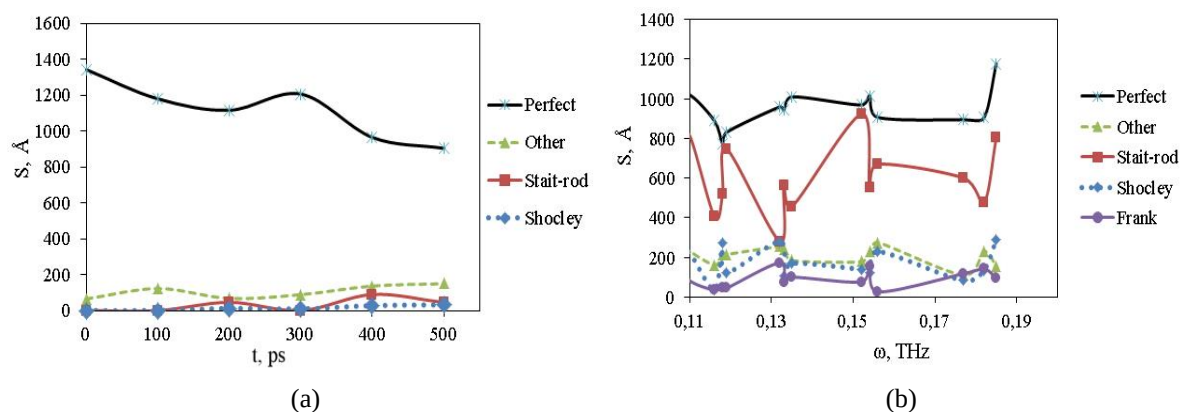


Figure 2. Change in the length of the dislocation segments upon annealing (a) to a temperature of 800 K, and depending on the frequency of the external harmonic effect (b) after 500 ps of the experiment.

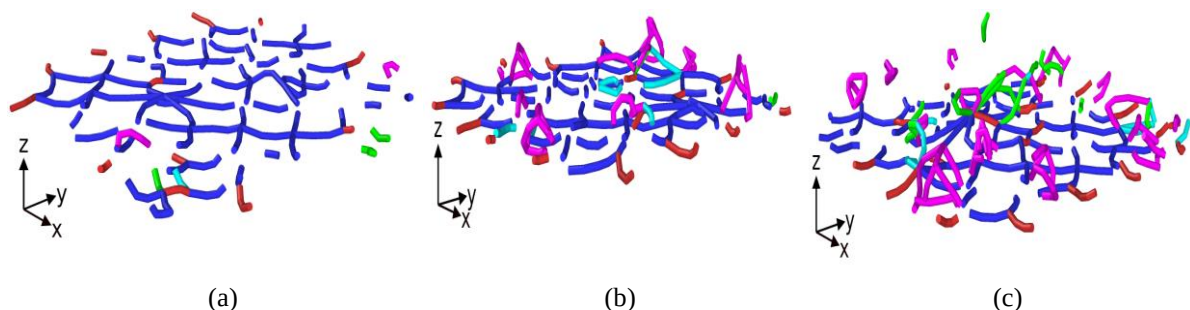


Figure 3. The dislocation structure under external harmonic action with an amplitude of 0.05 Å and a frequency of 0.1 THz: (a) after 10 ps, (b) after 250 ps, (c) after 500 ps. The color of the dislocation corresponds to their types in figure 1 (b).

Figure 3 shows the change in the dislocation structure upon external harmonic action. There was a transformation of misfit dislocations at the metal boundary into other types of dislocations with their displacement in Al. The formation of dislocations occurs in aluminum due to weaker Al – Al bonds. This generally leads to a lower melting point of aluminum. In figure 2 (b), peaks are clearly visible for a number of exposure frequencies. Their position on the frequency scale is related to the size of the simulated cell and is due to the presence of reflection waves from the network of dislocations and the surface of the bipartite bimetal. A decrease in the thickness of the Al layer led to their compaction, and an increase in the Al layer, respectively, to rarefaction.

As a result of external action, dislocation loops were formed based on Strair-rod type dislocations. Mostly, their nucleation occurred at the nodes of the network of misfit dislocations, as well as near the dislocation exit to the surface. An increase in the concentration of vacancies facilitates the release of dislocations to the surface of the Al crystal, as well as near the Ni-Al interface.

4. Conclusions

Using the molecular dynamics method, we study the behavior of misfit dislocations at the Ni-Al bimetal interface under external harmonic influence. The study was conducted in the case of the presence of point defects in the form of vacancies on the Al side. The vacancies promoted the formation of dislocation loops and the release of dislocations to the crystal surface.

A distribution is obtained for the types of formed dislocations depending on the frequency of the external harmonic effect. As a result of studying the dynamics of dislocation segments, it was found that the total number of segments and their total length remain the same. At the same time, misfit dislocations are transformed into other types: Strair-rod, Shockley, Frank. The results obtained can be useful in the production of bimetallic particles and their use as catalysts.

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References

- [1] Ellert O G, Tsodikov M V, Nikolaev S A and Novotortsev V M 2014 *Adv. Chem.* **83(8)** 718
- [2] Sanyal U, Therese D and Jagirdar Balaji R 2013 *Dalton Trans.* **42(19)** 7147
- [3] Eliana Misi S E, Ramli A and Rahman F H 2011 *J. Appl. Scien.* **11** 1297
- [4] Shirokorad D V, Kornich G V and Bug S G 2017 *Phys. Solid State* **59(1)** 189
- [5] Gavens A J, Van Heerden D, Mann A B, Reiss M E and Weihs T P 2000 *J. Appl. Phys.* **87** 1255
- [6] Wiemer M D, Braeuer J, Wunsch D and Gessner T 2010 *ECS Trans.* **33** 307
- [7] Kamaeva O V and Chernov V M 2002 *Phys. Solid State* **44(9)** 1676
- [8] Chernov V M and Persiyanova E I 2008 *Phys. Solid State* **50(4)** 649
- [9] Zagulyaev D V, Konovalov S V, Shlyarov V V, Anuchina E A, Komissarova I A and Gromov V E 2016 *IOP Conf. Series Materials Science and Engineering* **150(1)** 012038
- [10] Petukhov B V 2008 *Phys. Solid State* **50** 1438
- [11] Tschoop M A, Spearot D E and McDowell D L 2008 *Disloc. Solids* **14** 43
- [12] Barannikova S A, Li Yu V and Zuev L B 2019 *IOP J. Phys.: Conf. Series* **1129** 012004
- [13] Kamaeva O V and Chernov V M 2002 *Condensed matter and interphases* **2(4)** 316
- [14] Teplyakova L A, Kunitsyna T C and Koneva N A 2015 *IOP Conf. Series Materials Science and Engineering* **71(1)** 012064
- [15] Rabinovich M I and Trubetskov D I 2000 Introduction to the theory of oscillations and waves (Izhevsk: Scientific and Publishing Center "Regular and Chaotic Dynamics") p 580
- [16] Zakharov P V, Poletaev G M, Starostenkov M D and Cherednichenko A I 2017 *Lett. Mater.* **7(3)** 296
- [17] Cherednichenko A I, Zakharov P V, Starostenkov M D, Sysoeva M O and Eremin A M 2019 *Comp. Res. Model.* **11 (1)** 109

- [18] Zakharov P V, Eremin A M, Starostenkov M D, Lutsenko I S, Korznikova E A and Dmitriev S V 2019 *Phys. Solid State* **61(11)** 2160
- [19] Bayazitov A M, Korznikova E A, Shepelev I A, Chetverikov A P, Khadiullin K S, Sharapov E A, Zakharov P V and Dmitriev S V 2018 *IOP Conf. Series: Materials Science and Engineering* **447(1)** 012040
- [20] Poletaev G M, Novoselova D V, Tsellermaer V Ya and Kovalenko V V 2016 *Key Eng. Materials* **685** 8
- [21] LAMMPS Molecular Dynamics Simulator Retrieved from <http://lammps.sandia.gov/>