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MOLECULAR DYNAMICS STUDY OF PLASTIC DEFORMATION MECHANISMS NEAR THE INTERPHASE BOUNDARY IN TWO-DIMENSIONAL BIMETALLIC SYSTEMS

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Abstract. The atomic mechanisms of plastic deformation near the Ni-Al, Cu-Au, Ni-Fe coherent interphase boundaries in two-dimensional model are studied by the method of molecular dynamics. It is shown that plastic deformation near the interphase boundary is closely connected with misfit dislocations. Plastic shears and destruction of the bimetals are initiated near the misfit dislocations cores.

1. Introduction

Interphase boundaries, as well as grain boundaries, play an important role in the plastic deformation. It is known that plastic shears are often initiated at the interfaces (free surface, grain and interphase boundaries) [1, 2]. In [3-5], using molecular dynamics simulation, we showed that low-angle grain boundary dislocations play an important role in the diffusion and plastic shears formation near the boundaries at deformation.

Dislocations in the coherent interphase boundaries are formed not only as a result of disorientation of contacting crystals (as in the case of grain boundaries), but due to mismatch of lattice parameters of the phases (the so called misfit dislocations) [6, 7]. As grain boundary dislocations, misfit dislocations can act as sources of various defects: point and line defects, stacking faults, or, conversely, delay moving dislocations and absorb vacancies and interstitial atoms. Previously [8], it was found that the density of misfit dislocations largely affects the intensity of diffusion near the coherent interphase boundary.

Plastic deformation with the participation of phase boundaries plays a key role, such as, at the explosion welding. In this case, a strong bond of metals is being formed under high collision velocities of the order of 0.1-1 km/s. At such velocities, a strong plastic deformation takes place until a local melting in the contact area. In most cases, it was noted that the welding seam is obtained diffusionless, but of very high strength [9, 10].

This paper considers the research of plastic deformation mechanisms near the interphase boundary in the two-dimensional model by the method of molecular dynamics. As bimetals considered Ni-Fe, Au-Cu, Ni-Al. During the research process the attention was focused on the role of misfit dislocations during plastic deformation.

2. Description of the model

Molecular dynamics is a computer simulation of physical movements of atoms and molecules in the context of N-body simulation. The atoms and molecules are allowed to interact for a period of time, giving a view of the motion of the atoms. In the most common version, the trajectories of atoms and molecules are determined by numerically solving the Newton's equations of motion for a system of interacting particles. For the research we used own licensed computer software (MD2).

Packing of atoms in the molecular dynamics two-dimensional model was corresponded to the most densely packed (111) plane of fcc lattice. Interatomic interactions were described by Morse pair potentials:

$$\varphi_{AB}(r_{ij}) = D_{AB}\beta_{AB}e^{-\alpha_{AB}r_{ij}}\left(\beta_{AB}e^{-\alpha_{AB}r_{ij}} - 2\right),$$

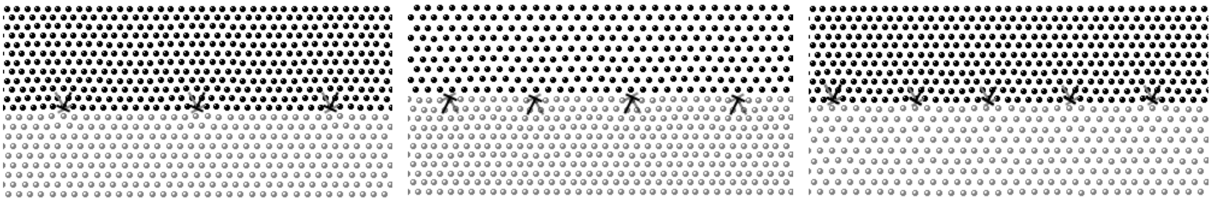
where α_{AB}, β_{AB}, D_{AB} - potential parameters determining the interaction of an atoms pair of A and B types; r_{ij} - distance between i and j atoms of A and B types. Potential parameters were taken from [11].

The interphase boundary was created in the middle of the calculation block, containing from 3000 to 8000 atoms. Various orientations of the boundary were considered. Time step of atoms motion integration in the molecular dynamics method in all experiments was equal to 10^{-14} s.

In this paper, two directions of deformation of the calculated block were considered: the tension-compression deformation perpendicular to the interphase boundary and along it. In the first case, the periodic boundary conditions along the boundary were defined (imitating the endless repetition of the calculation block along the boundary), across - the flexible, allowing the calculated block to change the volume (border atomic lines, perpendicular to the boundary, moved in a computer experiment as a single unit that excluded plastic shears formation from the free surfaces). In the second case, conditions across the boundary were defined free, allowing dislocations formed not only inside the block, but from the free surface.

Deformation in the model was set by two methods: by moving with constant velocity "clips" (border atoms) on opposite sides of the calculated block or by changing of interatomic distances along considered direction in the start configuration of calculation block.

After the bimetal creation the structural relaxation was performed, at the end of which the calculation block was cooled. In the relaxation process, during which conjugation of contacting metals occurred, misfit dislocations were being formed at the interphase boundary (Fig. 1). The dislocations were being formed as a result of lattice parameters mismatch and disorientation of contacting crystals. This type of dislocations (i.e. two dislocations having a single core) is characteristic of the (111) plane of fcc lattice. Such dislocations are also called "60-degree dislocations" [1]. In the following figures the dislocations will be represented by only one T-shaped icon.



a) b) c)

Fig. 1. Misfit dislocations in the interphase boundaries oriented along <110> direction in (111) plane of fcc lattice: a) Ni (top, black atoms) – Fe (bottom, gray atoms); b) Au (top, black atoms) – Cu (bottom, gray atoms); Ni (top, black atoms) – Al (bottom, gray atoms).

3. Tension-compression deformation perpendicular to the interphase boundary

When simulating of the collision of two metals with 0.1-1 km/s velocities, that takes place, for example, at explosive welding [9, 10], it was found that in this case most of the voids and unevenness at the boundary are filled, i.e. the contact area of the two phases at the atomic level is obtained large enough for a firm connection. In addition, at the collision at high velocity or at high compression of the metals perpendicular to the boundary plastic shears were formed, periodically repeated along the boundary. The period of shears repetitions was multiplied to the repeatability period of misfit dislocations (Fig. 2). With temperature increasing, the plastic shears appeared at the earlier stages of the collision.

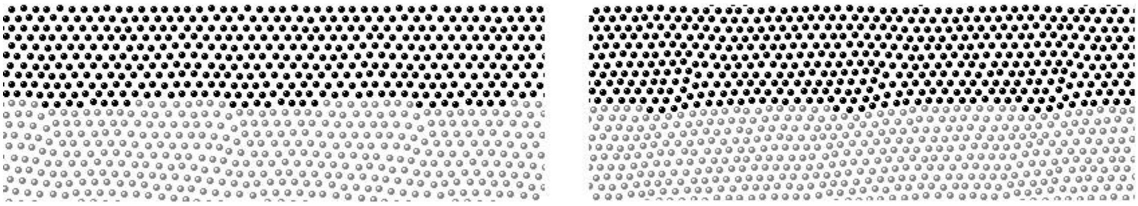


Fig. 2. Formation of periodic shears near the interphase boundary at the collision of Ni (top, black atoms) and Fe (bottom, gray atoms) along the direction perpendicular to the boundary at velocity 500 m/s.

At the tension perpendicular to the interphase boundary, the gaps appeared near the cores of misfit dislocations (Fig. 3). Depending on the bond energy of the atoms of different types, at the rupture the pores were formed near the dislocation cores or at the boundary (at relatively low bond energy, for example, at the boundary Ni-Fe) (Fig. 2a), or, at relatively high bond energy of the unlike atoms – near the cores, but in the metal which has a lower elastic modulus (Fig. 3 b, c).

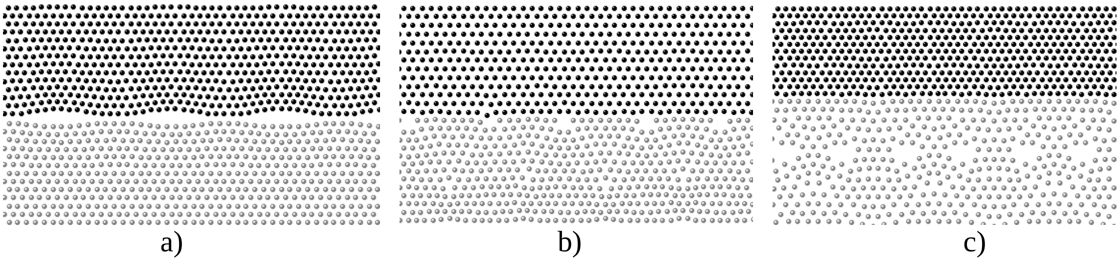
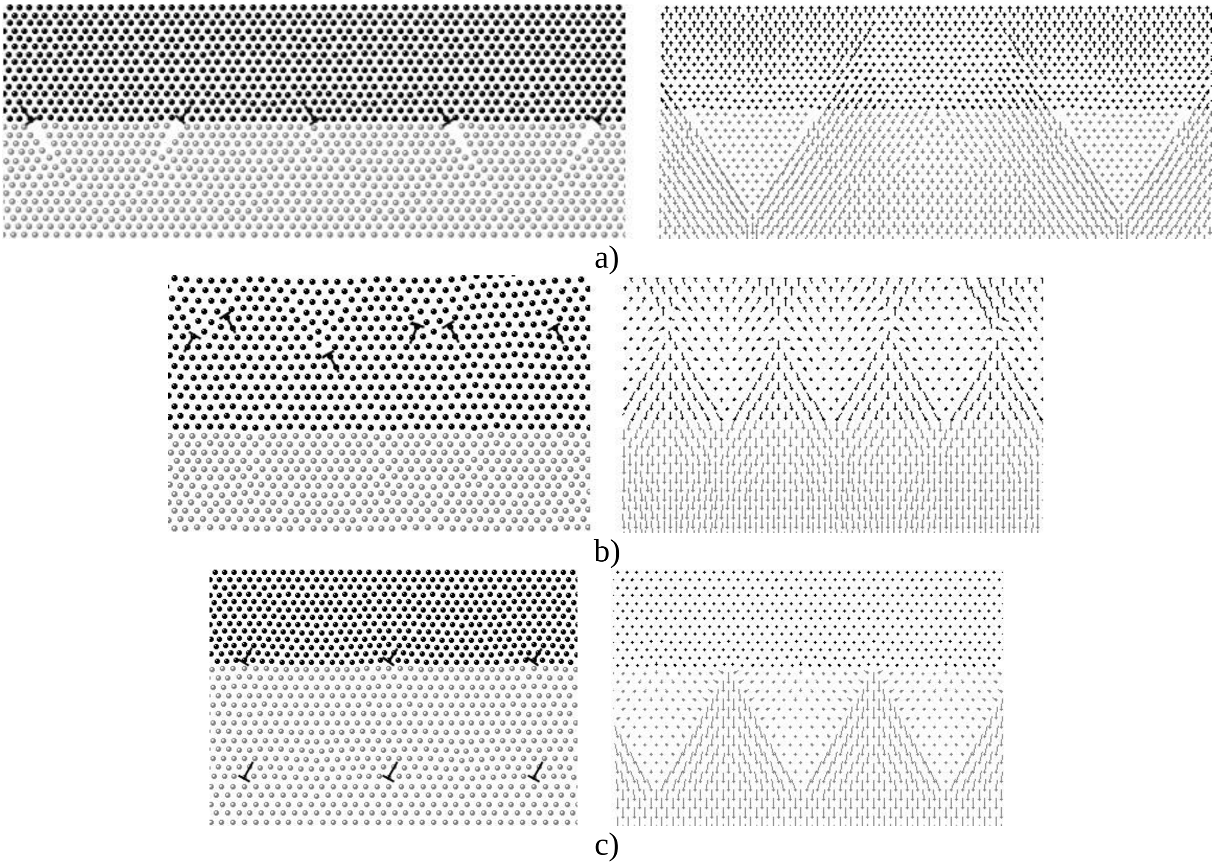


Fig. 3. Appearance of pores near the interphase boundary at the tension in direction perpendicular to the boundary: a) Ni (top, black atoms) - Fe (bottom, gray atoms), b) Au (top, black atoms) - Cu (bottom, gray atoms); a) Ni (top, black atoms) - Al (bottom, gray atoms).

4. Tension-compression deformation along the interphase boundary

Despite the fact that at the deformation along the interphase boundary there were free surfaces of both metals, plastic shears were started from misfit dislocations. Fig. 4 shows the location of the dislocations and atomic displacements in the calculation block at the initial stage of plastic deformation at tension along the interphase boundary. The figure shows that the plastic shears are initiated at the misfit dislocations and have wedge-shaped form. Mechanism of formation of plastic shears depends on the bond energy of the unlike atoms, on the ratio of the lattice parameters and on elastic moduli. Thus, the bonds breaking in Fe near dislocation cores is typical for the Ni-Fe boundary, whereupon the wedge-shaped shears are form in it (Fig. 4 a). In the case of the boundary Au-Cu, motion of the dislocations was occurred from the boundary to Au volume. The interphase boundary in Fig. 4 (b) does not contain the misfit dislocations – they all had migrated to Au. The reason for this is the difference of deformation of various metals at the same load, and on the contrary at the same deformation the internal stresses in various metals are different. Similar mechanism was observed at tension along the Ni-Al boundary (Fig. 4 c). In this case, half of the misfit dislocations had migrated to Al. In all considered bimetals plastic deformation at tension was started from metal which had a larger lattice parameter (lattice parameters for considered metals: Ni – 3.524 Å; γ-Fe – 3.656 Å; Au – 4.078 Å; Cu – 3.615 Å; Al – 4.050 Å [12]).



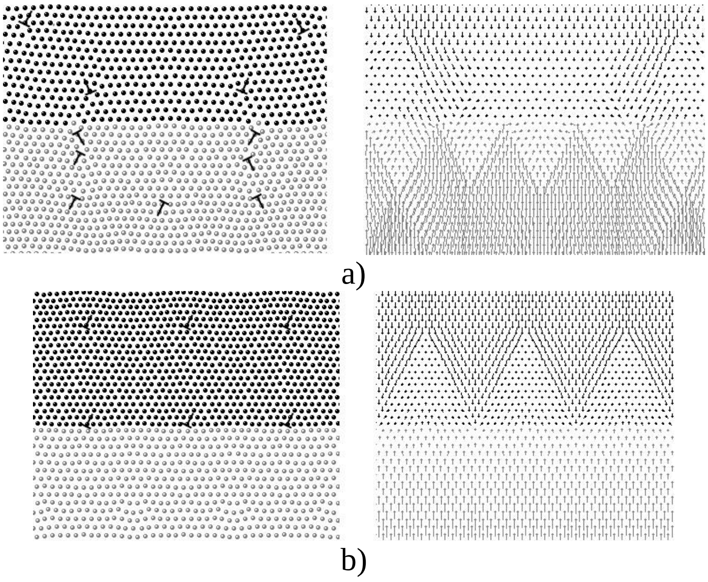
a)

b)

c)

Fig. 4. Plastic shears at tension along the interphase boundary. At the left - location of dislocations, at the right - image of the atomic displacements. a) Ni (top, black atoms) - Fe (bottom, gray atoms); b) Au (top, black atoms) - Cu (bottom, gray atoms); c) Ni (top, black atoms) - Al (bottom, gray atoms).

At the compression along the interphase boundary the similar wedge-shaped shears were observed, formed from the misfit dislocations (Fig. 5).



a)

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Fig. 5. Plastic shears at compression along the interphase boundary. At the left - location of dislocations, at the right - image of the atomic displacements. a) Au (top, black atoms) - Cu (bottom, gray atoms); c) Ni (top, black atoms) - Al (bottom, gray atoms).

However, during compression, in contrast to tension, they first were appeared, as a rule, in metal with a smaller lattice parameter. Apparently, this is due to the fact that at the same deformation in such metals higher internal stresses arise due to a relatively smaller interatomic distance. The density of misfit dislocations, as at the tension, at the boundary was decreased, - they were distributed at some distance from the boundary (Fig. 5). With the further development of the deformation the plastic shears were appeared in both metals, which extended from the free surface. At the same time they were correlating with the shears occurred from the misfit dislocations, and often had the same or multiple repetition period.

5. Conclusion

Thus, molecular dynamics study showed that plastic deformation near the interphase boundary is closely associated with misfit dislocations. Plastic shears and destruction of the crystal lattice are initiated near the cores of misfit dislocations. Atomic mechanism of the plastic deformation depends on the bond energy of atoms of different types at the boundary, on the ratio of the lattice parameters and on the elastic moduli. It was found out that at the tension along the boundary the plastic shears initially are formed from the misfit dislocations, as a rule, in a metal which has a larger lattice parameter. During compression, on the contrary, the plastic deformation begins in a metal with a smaller lattice parameter. Apparently, correlation with the lattice parameter is indirect. Therefore, if one of the contacting phases has a relatively low elastic modulus and sublimation energy, it is not excluded that the plastic shears will occur at compression and tension at the initial stage of plastic deformation in this phase.

Obtained results appear to be possible to check experimentally using microscopes with atomic resolution by examining interphase boundaries structure subjected to plastic deformation.

Acknowledgment

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References

[1] J.Y. Huang, Y.T. Zhu, H. Jiang, T.C. Lowe // *Acta Materialia* **49** (2001) 1497.
[2] H. Kawazoe, M. Niewczas // *Philosophical Magazine* **84** (2004) 381.
[3] R.Yu. Rakitin, G.M. Poletaev, M.S. Aksenov, M.D. Starostenkov // *Technical Physics Letters* **31** (2005) 650.
[4] M.D. Starostenkov, D.V. Sinyaev, R.Y. Rakitin, G.M. Poletaev // *Solid State Phenomena* **139** (2008) 89.
[5] M. Starostenkov, G. Poletaev, R. Rakitin, D. Sinyaev // *Materials Science Forum* **567-568** (2008) 161.
[6] Y.A. Tkhorik, L.S. Khazan, *Plastic deformation and misfit dislocations in heteroepitaxial systems* (Naukova Dumka, Kiev, 1990) (in Russian).
[7] G.M. Poletaev, M.D. Starostenkov // *Technical Physics Letters* **29** (2003) 454.
[8] G.M. Poletaev, L.M. Kobzar, N.A. Kulabukhova, M.D. Starostenkov // *Fundamental'nye Problemy Sovremennogo Materialovedenia* **4** (2009) 111 (in Russian).
[9] Y. Dor-Ram, B. Weiss, Y. Kommem // *Acta Metallurgica et Materialia* **27** (1979) 1417.
[10] V.V. Rybin, B.A. Greenberg, O.V. Antonova, L.E. Karkina, A.V. Inozemtsev, A.M. Patselov // *Welding Journal* **86** (2007) 205.
[11] A.I. Tsaregorodtsev, N.V. Gorlov, B.F. Demyanov, M.D. Starostenkov // *Fizika Metallov i Metallovedenie* **58** (1984) 336 (in Russian).
[12] Ch. Kittel, *Introduction to solid state physics* (New York, 2004).