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Molecular dynamics simulation of structural transformations in Cu-Al system under pressure

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Abstract. Aluminium-copper (Al–Cu) compounds are one of the most-studied precipitation-strengthened alloy systems. Mechanical properties of Cu-Al systems considerably dependent on the phase composition. Excellent properties primarily depend on the intrinsic microstructures formed during processing stages, particularly the precipitated phases or the so-called intermetallics, along with various defects and impurity segregation, have important influences on the composite strength. Study of fabrication techniques to obtain composites with improved mechanical properties, careful investigation of phase composition, dynamics and kinetics are of high importance. Molecular dynamics simulation is used to study on the atomistic level the process of formation of Al/Cu composite from two initially separated crystals by severe plastic deformation. The proposed model is the simplification of scenario, experimentally observed previously. However, even in such a simple model, understanding of the mechanisms underlying in the process of composite formation can be obtained.

1. Introduction

Aluminium-copper (Al–Cu) compounds are one of the most-studied precipitation-strengthened alloy systems. Mechanical properties of Cu-Al systems considerably dependent on the phase composition. Excellent properties primarily depend on the intrinsic microstructures formed during processing stages, particularly the precipitated phases or the so-called intermetallics, along with various defects and impurity segregation, have important influences on the composite strength. Study of fabrication techniques to obtain composites with improved mechanical properties, careful investigation of phase composition, dynamics and kinetics are of high importance.

In [1, 2, 3], the formation of in-situ composites is observed after high pressure torsion followed by annealing. Plastic deformation can be successfully used for the production of composites which can be produced by severe plastic deformation (SPD) processes resulting in grain size refinement to the nanoscale [4, 5, 6, 7, 8, 9]. To fabricate Al-Cu composite, plates of pure Al and Cu can be stacked and then processed by high pressure torsion. As it was shown, such hard phases as AlCu, Cu_9Al_4 and Al_2Cu can be obtained after treatment [1, 2, 3]. Moreover, to facilitate phase growth, annealing at 450 °C is applied to the as-processed composite.

In experiments, peculiarities of the structural and phase transformations cannot be clearly seen step by step but can be reproduced by various modeling techniques. Molecular dynamics simulation is a powerful tool for studying structure on an atomic level which allow tracking

different processes in metals during deformation or annealing. Numerous application of this method to study defects in metals, phase transformations, effect of external influences such as ultrasound or plastic deformation [10, 11, 12, 13, 14, 15].

In the present work, the dynamics of phase transformation in Cu-Al system are investigated by molecular dynamics. Pure pressure, pressure combined with shear deformation and annealing is used to facilitate the phase transformations.

2. Simulation details

The atomic structure of a bimetallic interface is presented in Fig. 1 in three projections. A bilayer model of Cu (blue atoms) and Al (red atoms) is created and assembled from two unrelaxed perfect crystals. The first atomic structure is formed by directly combining two perfect crystals by the home-made program. The periodic boundary conditions are applied in the x, y and z directions. Cu crystal has 55 periodicity-lengths along x, ∼100 Å, and 8 periodicity-lengths along z, 32 Å; Al crystal has 49 periodicity-lengths along x, ∼100 Å, and 7 periodicity-lengths along z, 32 Å. The distance between the two crystals is 2.8 Å. The structure is initially relaxed at 300 K to find a structural configuration with minimum potential energy.

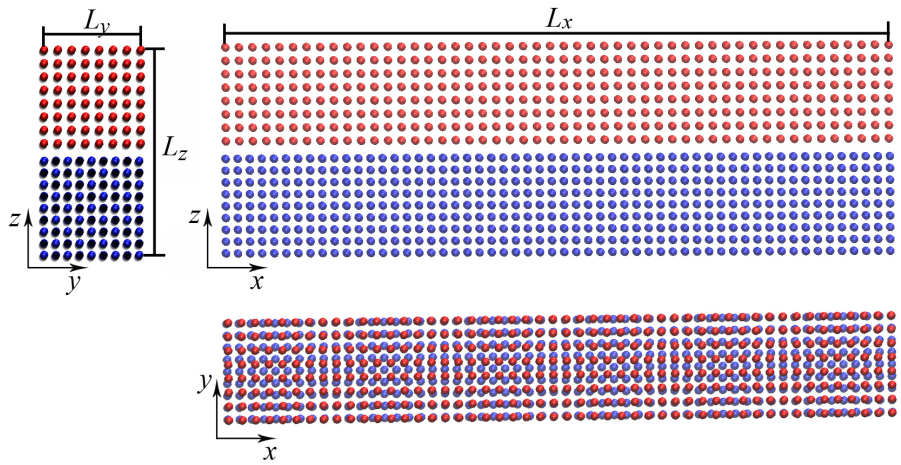

Figure 1. Simulation cell in three projections. Al atoms are shown by red, Cu atoms - by blue.

The simulations are carried out by molecular dynamics using the LAMMPS free simulation package. EAM interatomic potential [16] which gives a simple model for fcc metals and includes a long-range force is used. Previously, this interatomic potential was successfully used for simulation in [17, 18, 19]. To control the temperature equal to 300 K, Nose-Hoover thermostat is applied. Verlet algorithm to integrate the Newtonian equation of motion with an integration time-step of 2 fs is used.

To study the deformation behavior of Cu-Al system and phase formation, two types of loading are applied: (i) pressure along z axis and (ii) pressure along z combined with shear deformation σ_{xy}. Moreover, annealing at 300 °C and 450 °C is used to study the phase transformations in Cu-Al system. Three different strain rates are studied $\dot{\varepsilon}$=0.0001; 0.0005; 0.001.

In Fig. 2, pressure and potential energy as the function of strain for three strain rates are presented as well as the snapshots of the structure at t=250 ps (corresponding strain rate is mentioned). It is found that better to apply strain rate 0.0001 ps^{-1} which allows seeing much more diffusion acts in the structure (shown by green circles in Fig. 2c). Pressure-strain curves for $\dot{\varepsilon}$=0.001 ps^{-1} and $\dot{\varepsilon}$=0.0005 ps^{-1} are almost coincide which means that at both strain rates diffusion is blocked. Further, only $\dot{\varepsilon}$=0.0001 ps^{-1} is discussed.

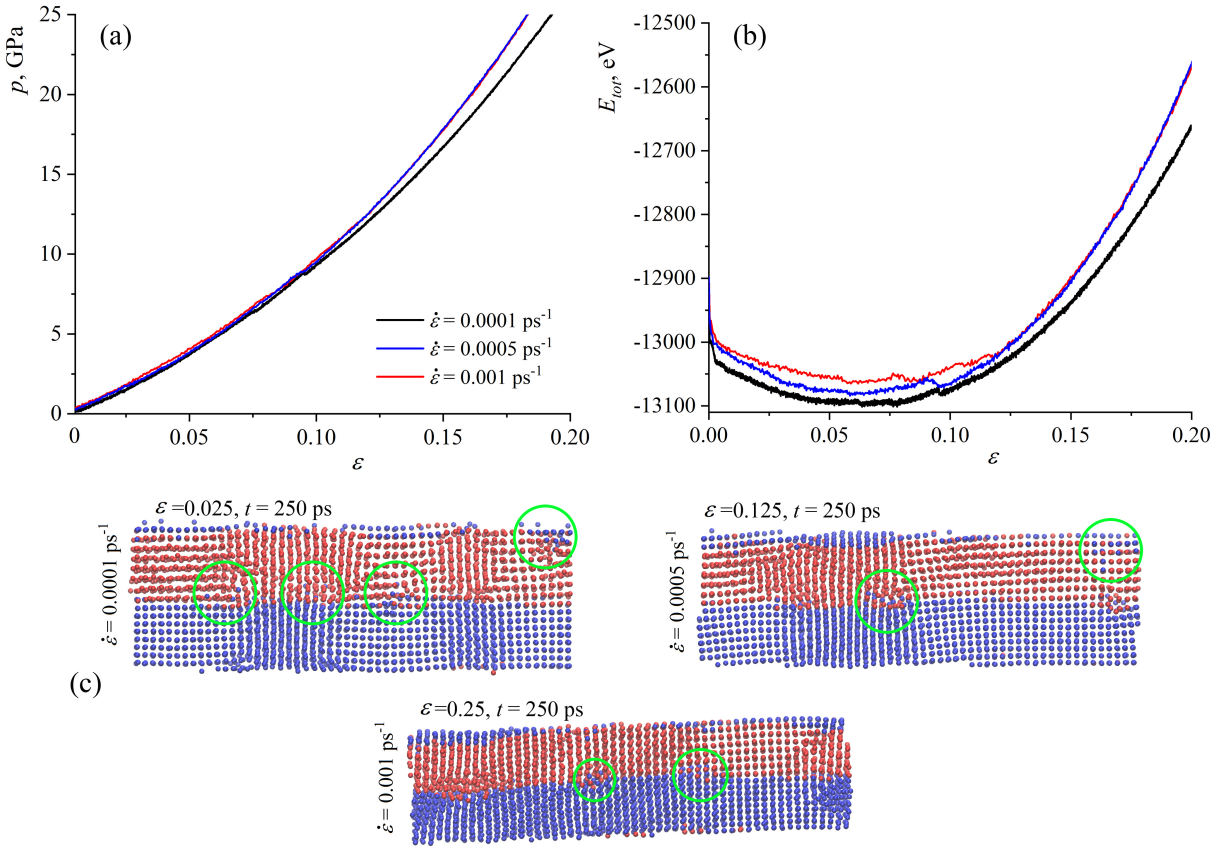

Figure 2. Pressure (a) and potential energy (b) as the function of strain for three strain rates. (c) Snapshots of the structure at t=250 ps for three strain rates. Al atoms are shown by red, Cu atoms - by blue. Green circles are shown to set aside region where mixing of the atoms took place.

3. Results and discussion

In Fig. 3, 4 stress-strain curves after uniaxial compression along z axis and pressure combined with shear stress τ_{xy}, respectively, are presented. For both cases, stresses σ_{xx}, σ_{yy} and σ_{zz} changing in a similar way, thus only σ_{zz} is shown. Shear stresses are also presented for comparison. To analyse the distribution of the stresses on each atom, snapshots of σ_{zz} distribution are presented for ε_{zz}=0.005;0.03;00.5;0.07 (Fig. 3) and ε_{zz}=0.005;0.03;00.5;0.07 (Fig. 4).

As can be seen from Fig. 3, high stresses σ_{zz}=27 GPa are achieved at ε_{zz}=0.2. Initially, the structure was relaxed with both positive and negative stresses equally distributed in both parts. Compression stresses increase continuously with an increase in pressure value. The same behavior is seen in Fig. 4, however at ε_{zz}=0.07 stresses are not so large and additional shear strain help to relax stresses in the structure. As can be seen, σ_{xx} on the atom is negative (compressive) mostly in Al part of the composite because of its softness even after ε_{zz}=0.05 for simple compression and ε_{zz}=0.03 for compression combined with shear. Stresses σ_{xx} on the atom are distributed in the same way.

In Fig. 5, snapshots of the structure in projection to xz plane at the initial state, after pressure along z axis at ε_{zz}=0.1, after pressure along z axis ε_{zz}=0.075 combined with shear are presented for Cu atoms only. The lower border of Cu crystal is shown above Al crystal because

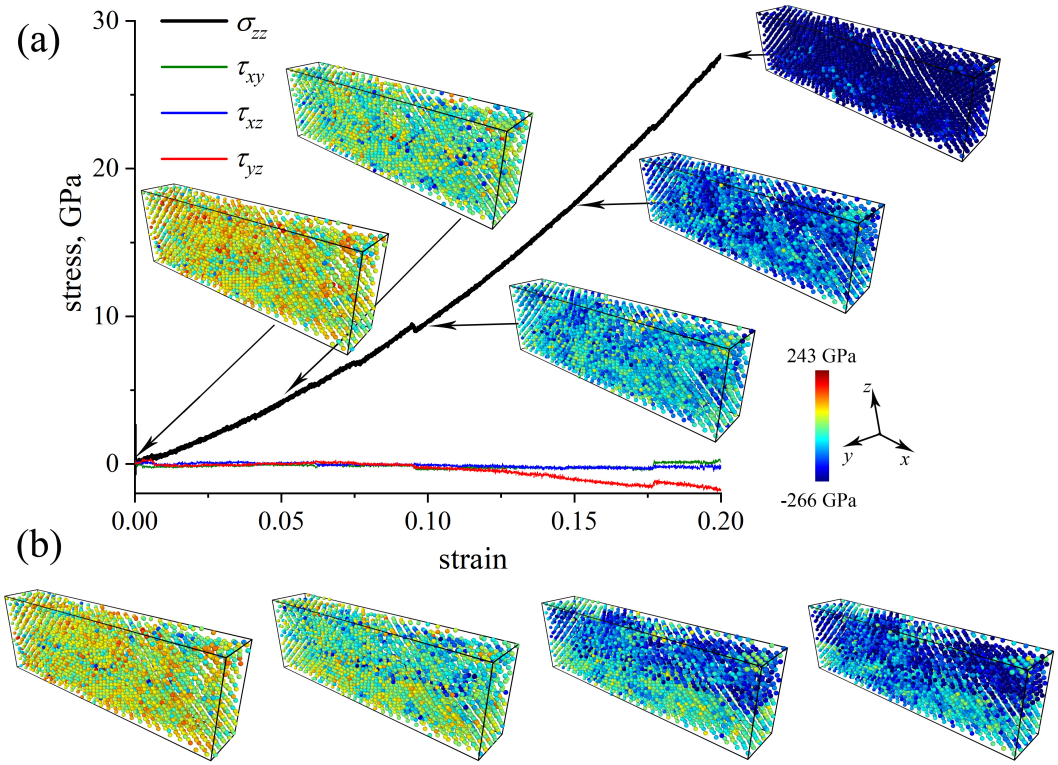

Figure 3. (a) Stress-strain curves after uniaxial compression along z axis. Distribution of the stress σ_{zz} (a) and σ_{xx} (b) on atom is also presented for ε_{zz}=0.005;0.05;0.15;0.2 (a) and ε_{zz}=0.005;0.05;0.15 (b).

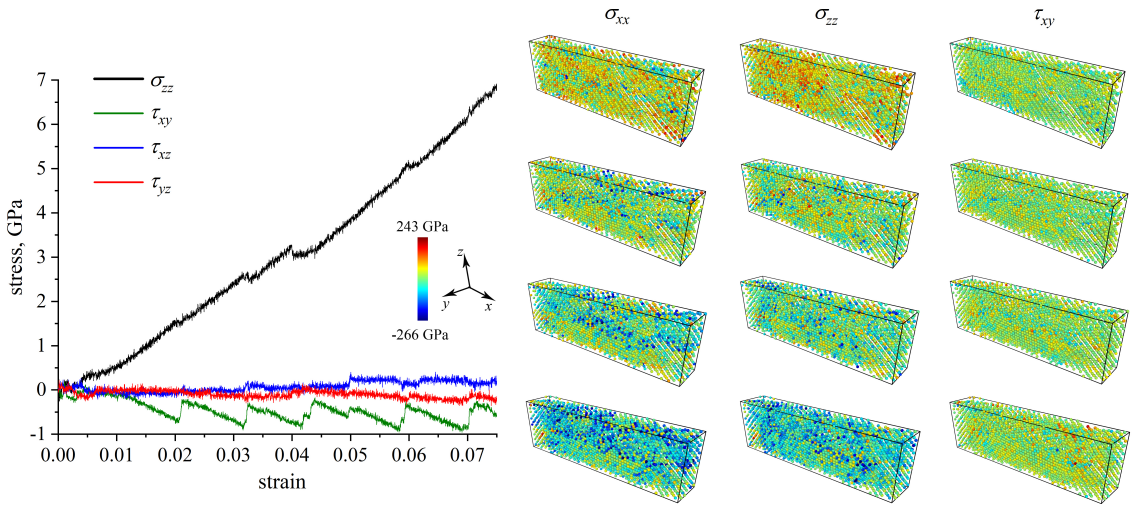

Figure 4. Stress-strain curves after uniaxial compression along z axis combined with shear stress τ_{xy}. Distribution of the stress σ_{xx}, σ_{zz} and σ_{xy} on atom is also presented for ε_{zz}=0.005;0.03;0.05;0.07.

of periodic boundary conditions. As can be seen, after uniaxial compression just several Cu atoms move towards Al crystal even at ε_{zz}=0.01 and σ_{zz}=10 GPa. However, as it is well-known in the experiment during high pressure torsion not only compressive strain is applied but shear

stain too. Thus, shear components can facilitate the mixture of the atoms on the borders of two metals. From the snapshots of the structure after ε_{zz}=0.007 and additional shear strain (Fig. 5 "pressure+shear") more atoms move towards Al crystal from the top and bottom parts of Cu crystal. It should be noted, that better results are achieved at much lower pressure ε_{zz}. As it was previously shown, severe plastic deformations can facilitate the formation of intermetallic phases, because materials after HPT diffusion coefficient considerably increases [20, 21, 22].

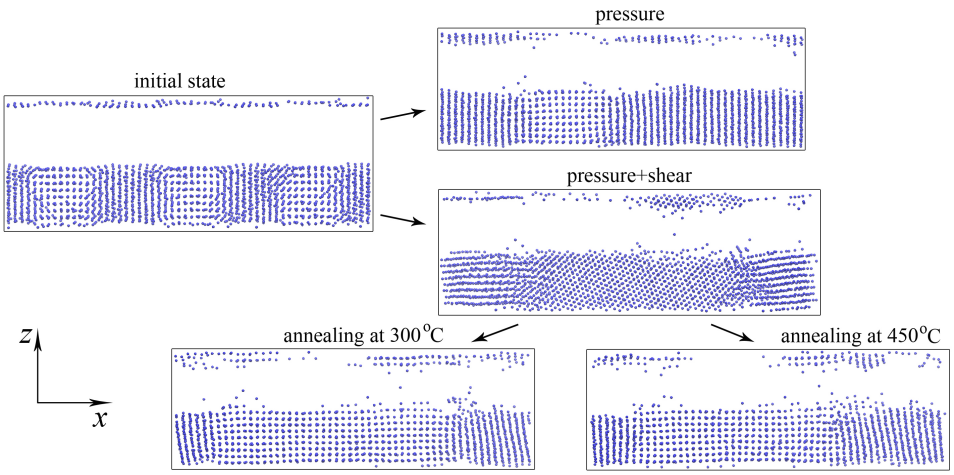

Figure 5. Snapshots of the structure at the initial state, after pressure along z axis at ε_{zz}=0.1, after pressure along z axis ε_{zz}=0.075 combined with shear and structures annealed at 300°C and 450°C. Only Cu atoms are shown.

As it is mentioned in [1, 2, 3], mixing of Al and Cu atoms took place after hydrostatic compression and much more new intermetallic phases were obtained after annealing. From Fig. 5, where snapshots after annealing are presented, the same scenario can be seen: Cu atoms probed deeper into the Al matrix. From the distribution of stresses inside the structure (Figs. 3,4), it can be seen that additional shear stress allows deforming the structure more uniformly. Such high pressure (30 GPa achieved at simple compression) will not lead to further structural transformations.

Although MD simulation has a lot of limitations and especially concerning the diffusion process, the proposed model clearly shows the effectiveness of high pressure torsion for improvement of atoms mixing in Cu/Al system. Obtained results are in good connection with the experimental works. Analysis of the atomic movement during composite fabrication can shed light on the understanding of the underlying mechanisms.

4. Conclusions

In summary, molecular dynamics simulation is used to study on the atomistic level the process of formation of Al/Cu composite from two initially separated crystals by severe plastic deformation. The proposed model is the simplification of scenario, experimentally observed previously in [1, 2, 3]. However, even in such a simple model, understanding of the mechanisms underlying in the process of composite formation can be obtained.

Two basic schemes are considered: uniaxial compression and compression combined with shear deformation. As can be seen, additional shear stress components considerably facilitate the diffusion process. Even better mixing of Al and Cu atoms was obtained after annealing at 450°C. The present work raised a number of issues such as (i) effect of boundary conditions;

(ii) effect of crystal size and (iii) required combination of values of shear and compressive strain which could be studied in further works.

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6. References

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