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Influence of copper inclusions on the strength of aluminum matrix at high-rate tension

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ABSTRACT

In this work, we perform the molecular dynamics (MD) investigations of Al–Cu nanocomposite strength in the conditions of a high-rate uniaxial tension. The investigated material is an Al matrix with spherical nanoinclusions of Cu. The obtained results show that the formation of voids leading to fracture begins inside the aluminum matrix near the interface between Al and Cu. From a viewpoint of the nanocomposite strength, the main effect of Cu inclusions is connected with the stress concentration that leads to an action of increased stresses inside the matrix near the interface with inclusions; these increased stresses are 1.2–1.3 times higher than the volume-average value of stress (for the temperature of 300 K). With the increase of temperature, the plastic relaxation becomes more active due to increased rate of dislocations generation that reduces the role of stress concentrators; the effect finally disappears at temperatures >700 K. A few atomic layers of aluminum remain on the copper inclusions after the fracture, which indicates good adhesion properties of the Al–Cu interface. We propose a continuum model of the nanocomposite fracture that is based on the equations of nucleation and growth of voids inside the aluminum matrix; the model takes into account the stress concentration around inclusions. A comparison with the MD results shows that the continuum model allows us to describe the rate and temperature dependences of the nanocomposite strength at least for strain rates $\geq 10^8$ s^{-1}. At moderate strain rates, the strength values that are calculated with the continuum model correspond to the experimental data for the aluminum alloy 2024 with the second phase precipitates.

1. Introduction

Composites with aluminum matrix reinforced with inclusions are one of the perspective types of composite materials for utilization in numerous industrial applications [1–3]. Such composite materials can have a greater hardness, a better specific strength, a higher wear resistance, an increasing creep resistance and a lower thermal expansion coefficient in comparison with the matrix material [1–6]. Another advantage of the composite materials with the aluminum matrix is the ease of their manufacture. They can be prepared by casting [7–9] or by powder metallurgy [4,10]. Size of inclusions in such composites ranges from tens of nanometers to hundreds of micrometers, and the volume fraction of inclusions at the same time ranges from a few to tens of percents. Copper inclusions can be used for production of nanocomposites on the basis of aluminum matrix; the copper is also an important component in various Al alloys. A number of experimental [11–16] and molecular dynamics [17,18] investigations of the mechanical and thermodynamic properties of the Al–Cu alloys were carried out over the past years. The heterogeneity of structure is a common feature of alloys and nanocomposites, which are distinguished mainly by the method of manufacture. Besides the method of production, alloys are generally characterized by a wider variety of sizes of inclusions and a more complex chemical composition. The presence of inclusions in the matrix obstructs the motion of dislocations that leads to an increase in yield strength. As a result, the alloy or the composite material is more rigid than pure aluminum.

Since the increase of shear strength often leads to a drop in tensile strength (embrittlement), it is interesting to examine how the presence of inclusions in aluminum matrix affects the tensile strength. Presence of the interfaces between inclusions and matrix may also reduce the tensile strength, because the threshold energy of the voids formation on these surfaces can be lower than that in a pure material due to poor adhesion of the copper and aluminum atoms. Another possible cause of the decrease in strength is the stress concentration near the inclusions. As a result of stress concentration, the local stresses inside the matrix around the inclusions can reach the tensile strength despite the fact that the average stresses in the material are lower than the tensile

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strength. For ascertainment of the mechanisms and regularities of fracture, and for estimation of the influence of inclusions on the tensile strength, a molecular dynamics (MD) investigation of Al–Cu composite fracture under the high rate tension was carried out in this work. The MD data were generalized by construction of a continuum model of fracture. The results may be useful for analysis of the strength of Al–Cu alloys with the precipitates of the second phase.

2. Molecular dynamics simulations

2.1. MD setup

Molecular dynamics simulations were carried out with using of the LAMMPS package [19] and the interatomic potential [20], which is an angular dependent potential (ADP)–generalization of the embedded atom method (EAM) potential. We compared the tensile strength of pure aluminum and composite material (aluminum with a spherical inclusion of copper with size in the range of nanometers). In the case of composite material, the MD model was prepared in the following way: a cube-shaped sample of single-crystal aluminum was created initially, whereupon, a sphere of the specified radius R was cut out from the center of this cube, and a spherical inclusion of the same radius made from single-crystal copper was put inside the pore. Both lattices, of surrounding aluminum and copper inclusion, were oriented in such a way that the lattices directions [100], [010] and [001] coincide with the cube faces. Overlapping of atoms was not observed in all investigated cases; at the same time, the contact between atoms of inclusions and surrounding matrix was fine, which was confirmed by additional simulations with an energy minimization procedure after the inclusion insertion: results with this additional procedure and without this procedure coincided with each other.

Uniform uniaxial tension with constant strain rate was modeled by the scaling of coordinates of atoms with the use of 'deform' command of LAMMPS. The uniaxial deformation along one of sample faces (in [001] direction) was examined since this type of deformation is realized under the action of a plane shock wave on material, for instance. Periodic boundary conditions were set at all boundaries of the system. In the case of composite, using of these conditions is equivalent to consideration of a system of identical periodically arranged inclusions with concentration d^{-3}, where d is the MD model size. Thus, the volume fraction of inclusions is $(4\pi/3)(R/d)^3$, where R is the inclusion radius. The system was deformed in a Nose–Hoover thermostat at the constant temperature and with the relaxation time of 0.1 ps (time step was 0.001 ps). Prior to deformation, the system was brought to thermodynamic equilibrium at the given temperature and atmospheric pressure during 100 ps; the Nose–Hoover thermostat and barostat were used at this stage.

The main part of calculations was carried out for a system with the size $50 \times 50 \times 50$ of the lattice parameters of aluminum, which corresponds to the initial length of the cube face about $d = 20$ nm, and the number of atoms in the model about 500,000. In most calculations, the inclusion diameter was equal to $2R \approx 8$ nm, which corresponded to a volume fraction of inclusions equal to 0.034. For investigation of the size effect in pure aluminum, a number of simulations with different systems (with the cube faces of 20, 30, 40, 50, 60, 70, 80 and 100 lattice periods) were performed. The calculated values of tensile strength for different systems vary in the range less than 1% (6.36 ± 0.02 GPa at temperature of 300 K and the tension rate of 10^9 s^{-1}) without any clear monotonic dependence on the system size. This fact indicates an absence of size effect in the considered case. The size effect is pronounced in the cases of nanopillars [21] and nanowires [22], it means, the systems

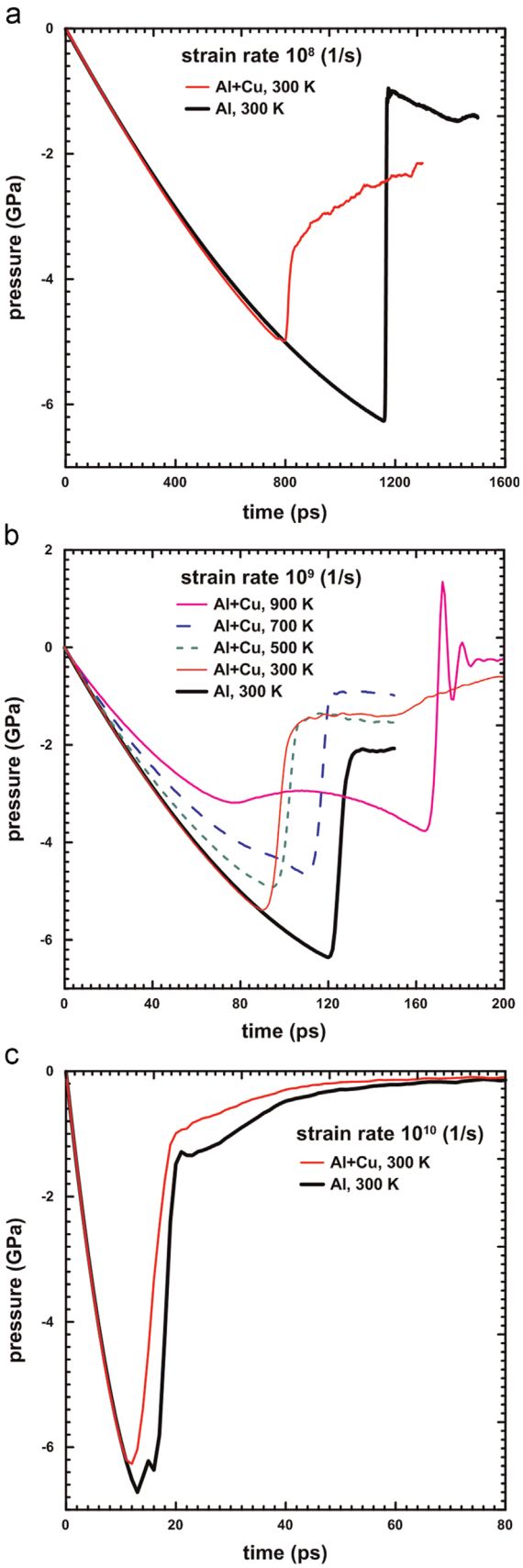

Fig. 1. The time dependences of pressure in pure aluminum and composite materials at various temperatures and strain rates. Strain rates are: (a) 10^8 s^{-1}, (b) 10^9 s^{-1}, and (c) 10^{10} s^{-1}. Calculations with LAMMPS package [19] and the ADP interatomic potential [20].