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DYNAMIC FRACTURE OF ALUMINUM AND IRON WITH NANOINCLUSIONS: MULTISCALE INVESTIGATION

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1 INTRODUCTION

At the present time nanocomposites, and alloys with aluminum matrix are widely used in various applications. They can have better properties (stiffness, specific shear strength, etc.) in comparison with a pure material of matrix. Heterogeneity is a common feature of alloys and nanocomposites. The presence of nanoinclusions in matrix obstructs the motion of dislocations that leads to an increase of shear strength [1]. On the other hand, the presence of inclusions [2] can decrease the tensile strength. For ascertainment of the mechanisms and regularities and for estimation the degree of influence of the inclusions on the strength, a molecular dynamics (MD) investigation of Al+Cu, Al+Ti and Al+Mg composites 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 aluminum alloys with the precipitates of the second phase

2 MD SETUP

MD simulations were performed using the parallel MD simulator LAMMPS [3] with interatomic EAM potentials [4-7]. All calculations were performed for a system with a size 50x50x50 of the lattice parameter of aluminum or iron (length of the cube face of approximately 20 nm). Radius of inclusion was equal 10 lattice parameters of aluminum of iron (radius of approximately 4 nm).

Inclusions were inserted in the following way: a sphere was cut out from the center of the system; thereafter, a sphere of monocrystalline inclusion was placed inside the pore. This procedure did not lead to an overlap of atoms. Quality of the contact between matrix and inclusion was examined by additional simulations with an energy minimization procedure after the inclusion insertion: the results obtained with this additional procedure and without this procedure coincide with each other.

Tension was along vertical direction in the main part of calculations. We consider aluminum matrix with copper, titanium and magnesium inclusions and iron matrix with nickel inclusion.

Inclusions can make metal weaker by different ways [2,8]: 1) stress concentration in

vicinity of strong and stiff inclusions (Cu or Ti in Al); 2) nucleation of voids inside inclusions made of a softer material compared with the matrix (Mg in Al); 3) nucleation of voids on the interface between matrix and inclusion inside the area of disordered material – it is realized for materials with close values of elastic and strength properties (Ni in Fe).

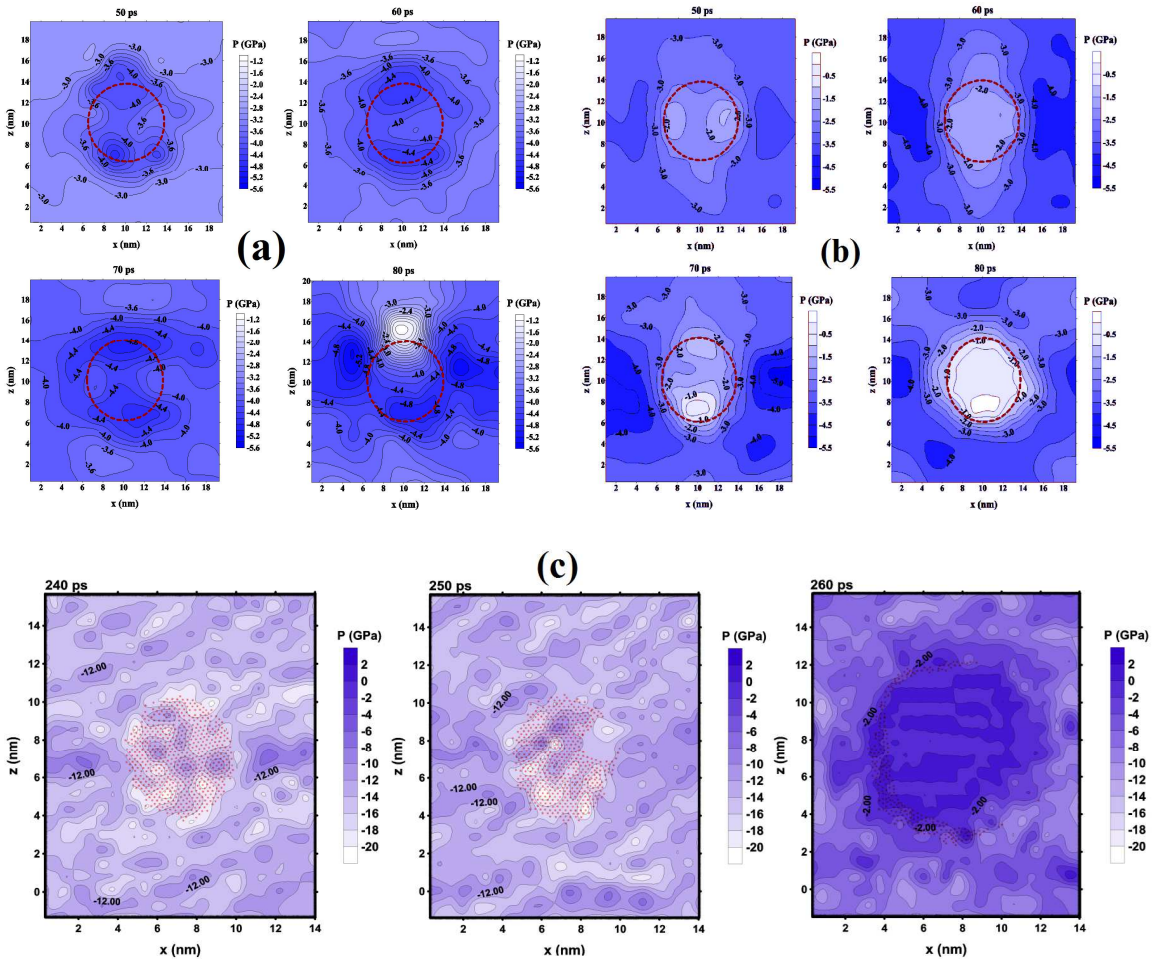

Figure 1: Distributions of pressure in the central cross-section of the systems: (a) Al+Ti; (b) Al+Mg; (c) Fe+Ni. Dashed circle in the center marks the position of the inclusion. Temperature is 300 K, strain rate is 10^9 s^{-1}.

3 CONTINUUM MODEL

MD results were used for construction of continuum model of fracture. The system of equations for a continuum model of fracture includes the continuity equation, the equation of motion and the equation for the internal energy. This system of equations takes into account formation and growth of the voids.

We suppose that all voids are spherical and they have the same radius in each point of material. In this case deformation tensor is diagonal and it is determined by the volume fraction of the voids, which, in turn, is determined by the void radius and concentration of the voids. Growth rate of void is controlled by the plastic deformation through motion of

dislocations in the void vicinity [9]. The equation of growth rate of void and the kinetic equation for total scalar density of dislocation in the void vicinity are described in the work [10-11].

Void nuclei arise within the areas of intersection of the stacking fault planes, which can exist initially or be formed in the course of deformation before the fracture beginning. Therefore the energy of the void nucleation is less, then that in the case of ideal lattice. We are taking it into account by introducing the reduction factor. The nucleation rate is written in typical manner.

4 RESULTS

Figure 2 shows the comparison of MD results (solid lines and symbols with error ranges), results of the continuum model of fracture (dash lines) and results of experiment (olive stars) [12]. Tensile strength versus strain rate is presented for the cases of pure aluminum and aluminum with different inclusions.

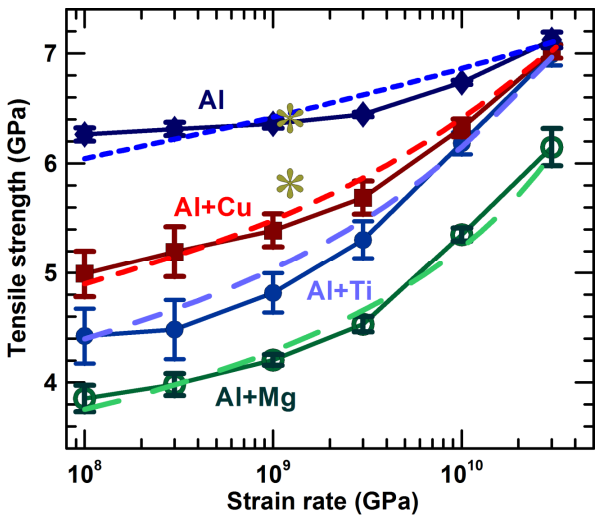

Figure 2: Comparison of MD results (solid lines and symbols with error ranges) with results of the continuum model of fracture (dash lines) and results of experiment (olive stars) [!!!!!].

At high strain rate difference between strength of pure aluminum and aluminum with inclusions decreases. It is accompanied by more intensive nucleation of voids in the main bulk and less role of specific areas.

5 CONCLUSIONS

- We consider using MD simulations three different mechanisms of reduction of the tensile strength of a material with inclusions in comparison with a pure material of matrix.
- We are developing method to construct tensile fracture models for pure metals and

alloys with maximal using MD data for elimination of fitted constants.

- A comparison with the MD results shows that the continuum model allows us to describe the rate dependences of the nanocomposite strength at least for strain rates ≥ 0.1/ns.

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