Tensile strength of Fe–Ni and Mg–Al nanocomposites: Molecular dynamic simulations

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Abstract. In this work, molecular dynamic simulations of the tensile strength of Fe–Ni and Mg–Al nanocomposites in the conditions of high-rate uniaxial tension were carried out. Two different mechanisms of fracture were identified. In the case of nickel inclusion in iron matrix, the fracture begins on the interface between the inclusion and the matrix, a formed void penetrates both into the inclusion and into the matrix; presence of inclusion reduces the tensile strength. In the case of aluminum inclusion in magnesium matrix, fracture takes place into magnesium matrix and does not touch the inclusion; presence of inclusion has practically no effect on the tensile strength. Molecular dynamic simulations were carried out in a wide range of strain rates and temperatures.

1. Introduction
Nanocomposites with magnesium and iron matrix and alloys based on magnesium and iron are perspective materials in various applications [1]. Interest in magnesium alloys and composites is due to their high rigidity and specific strength [2, 3]. Interest in iron alloys and composites is explained by their wide application.

A common feature of nanocomposites and alloys is the heterogeneity of their structure on nanoscale. At present, a number of papers are devoted to the experimental study of fracture of metals at high strain rates [4–6]. Therefore, the study of fracture at a nanoscale is an actual problem. The presence of inclusions in matrix obstructs the motion of dislocations that leads to an increase of shear strength [7]. On the other hand, the presence of inclusions [8] can decrease the tensile strength. The purpose of our work is to investigate the effect of nickel inclusions on the tensile strength of iron matrix and aluminum inclusions on the tensile strength of magnesium matrix. These materials of inclusions are chosen because they are most used in magnesium and iron alloys.

Earlier, we investigated the mechanisms of fracture in the case of considerable difference in the elastic moduli of inclusions and matrix [8,9]. Therefore, the case of close values of the elastic moduli of inclusion and matrix that takes place for nickel inclusion in iron matrix provokes an additional interest.

Also, magnesium matrix has hcp lattice and, in contrast to iron matrix with a bcc lattice, should exhibit pronounced anisotropic properties at tension along different axes. Therefore, comparing the fracture of magnesium and iron matrices is interesting from the point of view of determining the influence of matrix anisotropy on the process of fracture.
Figure 1. Histories of pressure in pure iron, nickel and Fe–Ni composite: uniaxial tension with the constant strain rate of $10^9$ s$^{-1}$ at the constant temperature of 300 K.

Figure 2. Histories of pressure in pure Al and Mg as well as in Mg–Al composite (MgAl): uniaxial tension with the constant strain rate of $10^9$ s$^{-1}$ at the constant temperature of 300 K. Simulation results of tension along each axis are presented for pure Mg and MgAl system.

2. Molecular dynamics setup
Molecular dynamic (MD) simulations were performed using the parallel simulator LAMMPS [10] with interatomic potentials [11, 12] for the cases of the nickel inclusion in the iron matrix and the aluminum inclusion in the magnesium matrix, respectively. Software package OVITO [13] was used for visualization of MD simulation results.

We considered the samples of pure iron, pure magnesium and also the iron and magnesium matrixes with spherical nickel and aluminum inclusions, respectively. In all cases, we initially specified the samples of monocrystalline iron (bcc lattice) or magnesium (hcp lattice) of cubic shape (with a cube face length denoted as $d$), which were oriented that the lattice directions ([100], [010], [001] for the iron; [2110], [0110], [0001] for the magnesium) were coincided with the cube faces (with the coordinate axes $x$, $y$ and $z$).

A sphere with a specified radius $R$ was cut out from the center of the system (in the iron or magnesium cube), thereafter, a sphere of the monocrystalline nickel or aluminum (fcc lattice) of the same radius was placed inside the pore. The lattices of the nickel and aluminum inclusions were oriented in such a manner that the lattice directions [100], [010] and [001] were coincided 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.

Periodic boundary conditions were set for all boundaries of MD sample that is equivalent to consideration of a system of identical, periodically arranged inclusions with concentration $\sim d^{-3}$. For the cases of pure iron and Fe–Ni composite, all calculations were performed for a system with
The initial radius of inclusions $R$ was equal to 10 lattice parameters of iron (about 2.9 nm) and 12 lattice parameters of magnesium (about 4 nm).

A uniform uniaxial tension with a constant strain rate was modeled with using the “deform” command of LAMMPS that corresponds to the substance expansion under its own inertia. This type of deformation is realized under the action of a plane shock wave on material, for instance. The system was deformed in a Nose-Hoover thermostat at the constant temperature and with the relaxation time of 0.1 ps. The system was brought to thermodynamic equilibrium at the given temperature and atmospheric pressure during 100 ps before the deformation; the Nose-Hoover thermostat and barostat were used at this stage.

3. Results and discussion

Figures 1 and 2 show typical histories of pressure for the Fe–Ni and Mg–Al nanocomposites and for pure components of these systems. The pressure decreases monotonically with time at initial stage of tension. The curves for pure iron, pure nickel and Fe–Ni composite are practically identical on this stage (see figure 1). This fact indicates the close values of elastic modules of
Figure 4. Dynamics of the void growth in Mg matrix with Al inclusion; the temperature is 300 K, and the strain rate is $10^9$ s$^{-1}$. Light red dots show Al atoms; dark blue dots show Mg atoms with the value of the centrosymmetric parameter more than 20 (atoms in vicinity of lattice defects) and with coordinate $x \leq L_y/2$, where $L_y$ is the size of MD system along y axis (in the faraway half of MD system).

Figure 5. Strain rate dependences of tensile strength at uniaxial tension at the constant temperature of 300 K: (a) pure iron, pure nickel and Fe–Ni composite; (b) pure magnesium, pure aluminum and Mg–Al composite.
Fracture of materials in all cases (see figures 1 and 2) begins at the achievement of a critical value of negative pressure; it consists in the formation and growth of voids. The material between the voids is being compressed that leads to a rapid relaxation of the tensile stress and pressure growth. The presence of inclusions in all calculations reduces the value of tensile strength of the systems in comparison with tensile strength of the matrix materials.

Figures 3 and 4 show the dynamics of void formation in Fe–Ni and Mg–Al nanocomposites at the strain rate $10^9$ s$^{-1}$ and temperature 300 K. These figures illustrate two different mechanisms of fracture. In the case of Fe–Ni nanocomposite (figure 3) the void formation begins in the area of disordered atoms near the interface between inclusion and matrix. It is caused by the close values of elastic moduli of inclusion and matrix. The formed void penetrates both into the matrix and into the inclusion and continues to grow until the material will be completely fractured. In the case of Mg–Al nanocomposite (figure 4) the void formation begins into the magnesium matrix both directly near the inclusion and on a distance from the inclusion. It is caused by the lower value of elastic moduli of magnesium matrix in comparison with the elastic moduli of aluminum inclusion.

Figures 5 and 6 show the strain rate and temperature dependences of the tensile strength in Fe–Ni and Mg–Al nanocomposites. The presence of nickel inclusion in the iron matrix leads to a significant decrease in the tensile strength in the investigated range of strain rates in comparison with the matrix material, figure 5(a). Decrease in strain rate, figure 5(a), and increase in temperature, figure 6(a), lead to a significant decrease in tensile strength of pure metals and Fe–Ni composite. The presence of aluminum inclusion in the magnesium matrix has practically no effect on the tensile strength in comparison with the matrix material and is determined by the strength of the matrix, figure 5(b). Both the strain rate, figure 5(b), and temperature, figure 6(b), dependences are weaker in this case in comparison with the Fe–Ni system.
4. Conclusions

With the use of MD simulations, in terms of nickel inclusion in the iron matrix and aluminum inclusion in the magnesium matrix, we examined two different mechanisms of influence of these inclusions on tensile strength in comparison with a pure material of matrix without inclusions. The first mechanism is connected with a stress concentration in magnesium matrix near a stiff and strong aluminum inclusion. The fracture occurs inside the matrix and does not touch the inclusion. Such mechanism is considered in [8,9] for the case of copper inclusions in aluminum matrix, in the present work it is realized for aluminum inclusions in magnesium matrix. The second mechanism is connected with atoms which are disordered along surface of nickel inclusion in iron matrix; in this case, the less energy is required for the voids formation in the area near the inclusion surface. The fracture begins inside this area of disordered atoms and thereafter propagates into the matrix and inclusion.

The tensile strength of Fe–Ni and Mg–Al systems is calculated at varied strain rates (in the range from 0.1 to 30 ns\(^{-1}\) at the temperature) and varied temperatures (in the range from 300 to 1500 K at the strain rate ns\(^{-1}\)).

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