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Weak increase of the dynamic tensile strength of aluminum melt at the insertion of refractory inclusions

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ABSTRACT

We investigate the influence of refractory inclusions on the tensile strength of metal melt with the use of the molecular dynamics simulations by an example of Ti inclusions in Al melt. It is found that the strength of melt with a low volume fraction of inclusions is close to the strength of pure melt, while the increase of volume fraction provokes the higher system strength. This increment of the tensile strength does not exceed 10% at the volume fraction growth up to 0.5. The reason of the observed hardening consists in the presence of stiff unmelted inclusions leading to an increase of the strain rate in the molten aluminum around the inclusions in comparison with the strain rate of the system as a whole, while the dynamic strength rises together with the strain rate increase. Form and orientation of inclusions do not influence the tensile strength; the volume fraction of inclusions is a sole important parameter.

1. Introduction

Expanded state of substance at negative pressure is unstable with respect to the nucleation and growth of voids. Increase of the volume of voids reduces the tensile stresses. As a result, the substance loses a possibility to resist further tension and can be fragmented. This process is the tensile fracture; the maximal absolute value of the negative pressure reached in substance during tension is the tensile or spall strength. The tensile strength increases together with shortening of the holding time of substance in the expanded state, it means, together with the strain rate increase [1,2]. The expanded state in dynamic mode of loading can be realized both in solids [1,2] and liquids [3–5] including metal melts [4,5]. Expanded state of metal melt can arise during fast expansion of an initially solid target, which is heated and melted by an ultra-short pulse of powerful laser irradiation [6,7] or high-current electron beam [8]. Another possibility consists in reflection of a compression pulse (a shock wave followed by an unloading wave) from a free surface of melt [9,10], when the compression pulse transforms into an expansion wave. Decay of the expanded state of liquid goes through formation and growth of voids as well; this process is typically referred as cavitation. Thus, one can talk about the tensile strength of melt in the dynamic conditions even it is not usual in the quasi-stationary case. The value of the tensile strength of metal melt is of interest in connection with possible formation of molten layers in the prospective power generating systems, as well as with the problems of coating and production of nanoparticles using the laser or electron-beam ablation.

In paper [5], we performed the molecular dynamics (MD) investigation of the tensile strength for several pure metals. The parameters of the continuum model of melt fracture were fitted by comparison with MD results, and this continuum model was applied for simulation of the high-current electron beam action on metals. Obtained values of the tensile strength of pure melts slowly decrease together with the strain rate reducing and occur in the range of several Gigapascals [5], which is comparable with the tensile strength of solid metals [11]. This result raises the question about how various initial heterogeneities, such as pre-existing pores or inclusions, influence on the tensile strength of melt and in what degree they can reduce the strength. It was shown in [11], that the pre-existing pores are rapidly healed due to the action of surface tension, and, thus, do not influence. The influence of foreign inclusions on the melt strength remains the question of considerable interest. In the case of solid metals, nanoinclusions made of a stiff and strong material play the role of obstacles for dislocation slip, and, thus, increase the yield strength that is a well-known result used in the particulate reinforced composites. On the other hand, they play the role of stress concentrators and, thereby, decrease the tensile strength of material in comparison with pure

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metal [12]. This effect of the material softening (in the sense of tensile strength) due to the presence of inclusions takes place even at low volume fraction of inclusions, which can be about or less than 1%, but the effect decreases together with the temperature growth [12]. Objective of present work consists in the MD investigation of the influence of refractory inclusions on the tensile strength of metal melt, as well as the analysis of causes and mechanisms of this influence.

2. MD setup

We considered aluminum melt with titanium inclusions at the temperature of 1100 K, which is higher than melting temperature of aluminum (933 K), but lower than the temperature of polymorphic transition from HPC α-Ti to BCC β-Ti (1156 K). MD simulations were performed with the help of molecular dynamics simulator LAMMPS [13] and with using of the interatomic potential [14], which is based on the formalism of the embedded atom method (EAM) [15]. Table of this potential was taken from the interatomic potentials repository [16]. Analysis of crystalline structure was preliminarily performed for MD samples of pure titanium and aluminum, as well as aluminum samples with titanium inclusions with the use of Adaptive Common Neighbor Analysis (a-CNA) [17], which is realized in the OVITO package [18]. This analysis showed that aluminum was in the molten state, while titanium remained solid and had HCP lattice (α-Ti). This conclusion was confirmed by the presence of shear stresses in pure titanium and the absence of shear stresses in pure aluminum at uniaxial tension of corresponding samples at the temperature of 1100 K.

A uniform uniaxial tension of MD system with a constant strain rate was modeled by scaling of atoms coordinates with using the command "deform" of LAMMPS that corresponds to the substance expansion under its own inertia. Qualitatively similar uniaxial strain is applied to substance after reflection of a plane shock wave from a plane free surface or during expansion of a substance layer heated by electron or laser beam. In spite of uniaxiality, there are no shear stresses, and only spherical component of stress tensor (pressure) acts in the system due to fluidity of melt. Periodic boundary conditions were set for all boundaries of MD system. The system was in the Nose–Hoover thermostat at the constant temperature of 1100 K during the deformation. The tensile strength of pure aluminum was investigated on the system that contained half a million atoms and was cubic initially. As it was shown in [12], there is no size effect for pure aluminum because the periodic boundary conditions make the problem statement equivalent to an infinite and uniform bulk sample without free boundaries. The aluminum melt was kept in thermostat and barostat at the test temperature and the pressure of 1 bar during 50 ps prior to tension.

The titanium inclusions in the aluminum melt were prepared by the following way. At first, we cut out a pore with sizes that were on 0.2 nm larger than the corresponding inclusion sizes in each direction. Thereafter, an inclusion made of a monocrystalline α-Ti with the standard HCP lattice was placed inside the pore, so that there was a narrow gap between the inclusion and the cavity surface. This gap was eliminated by means of the sample compression in the barostat at the pressure, which linearly decreased from 10 GPa down to 1 bar during the time interval of 50 ps with subsequent relaxation at the pressure of 1 bar during the next 50 ps. This preparation was done at the constant temperature that was equal to the temperature of the following tests. This procedure allowed us to exclude the overlap of atoms and provide the contact between Ti and Al atoms. Spherical inclusions (Fig. 1(a)) were investigated in the main bulk of calculations, while additional calculations were performed for inclusions in the form of rectangular parallelepiped (plate) with wide section perpendicular (Fig. 1(b)) and parallel (Fig. 1(c)) to the direction of tension (z axis) in order to test the dependence on the inclusion form. Sizes of inclusions varied in such range that the maximal volume fraction of inclusions reached 0.48; spherical inclusions almost contacted each other in this case. The volume fraction of inclusions was calculated by means of partition of the system on subregions and analysis of the fraction of Al and Ti atoms in each of subregions.

Several (from 4 to 10) MD trajectories were simulated in the same conditions of deformation in order to make a statistical analysis; the initial state of system was varied by setting different initial distributions of the atoms velocities. An average over MD trajectories value of strength was calculated, as well as the error range (the straggling of the tensile strength) that was estimated as for a direct measurement.

3. Results of MD simulations and analysis

Fig. 2 shows typical time profiles of the average pressure in the MD system. Tensile deformation leads to a decrease of the substance density and, as a result, to a monotone drop of pressure in the initial stage. The process of fracture starts at a certain value of negative pressure by means of nucleation and growth of voids. In the case of melt with inclusions, the voids arise and grow only inside the melt and do not touch the inclusions; the positions of voids do not correlate with the position of the interface between the inclusions and melt. The growth of voids initially decelerates the decrease of true density of substance between the voids, as well as the pressure decrease in the system; thereupon, it leads to increase of the true density and pressure. Minimum of pressure corresponds to the moment, at which the growth rate of volume of voids equalizes the growth rate of the system volume. The absolute value of this minimal (negative) pressure is the dynamic tensile strength P_S at the given conditions of deformation (temperature and strain rate). Subsequent growth of voids leads to relaxation of the expanded state and to fluctuations of the system pressure around the zero level. Further tension of the system results in the material fragmentation. We consider the initial stage of fracture and calculate the value of tensile strength P_S.

Voids in a monolithic material nucleate due to thermal fluctuations; it is a stochastic process [5]. Fig. 2 shows several MD trajectories that differ by initial distributions of thermal velocities of atoms. MD trajectories completely coincide till the beginning of fracture: there is a monotonic decrease of pressure along the same line. The moments of deviation from this line correspond to the voids nucleation and differ for the various MD trajectories; this is a manifestation of the probabilistic nature of the nucleation process. There is also a difference in the values of minimal pressure (the tensile strength P_S) and in the following behavior of systems.

As a first step, we verified the used interatomic potential [14] by comparison of MD results with the experimentally defined values of the tensile strength of solid [1] and molten [4] aluminum for the strain rate of 10^9 s^{-1}, which is directly accessible to MD simulations. In order to reach so high strain rate, an irradiation of thin aluminum foils by femtosecond pulses of powerful laser irradiation was performed in these experiments [1,4]; the values of strength were estimated from the analysis of the time profiles of the back surface velocity. For verification of the potential, a temperature dependence of the tensile strength was calculated for pure aluminum within the temperature range from 300 K up to 3000 K (the strain rate was 10^9 s^{-1}); the results are shown in Fig. 3 in comparison with the experimental data [1,4]. The calculated values lie near the lower edges of the experimental intervals for both solid [1] and molten [4] aluminum. The error ranges for MD results are calculated on the basis of several MD trajectories as for results