Molecular dynamics study of the nucleation rate of nanopores in aluminum at a negative pressure

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Abstract. The rate of a homogeneous nucleation of nanovoids in expanded aluminum is researched in this work. Typical lifetime of the system in a metastable state at a negative pressure as well as coefficients of surface tension and nucleation frequency at the temperatures 300 and 500 K are obtained with the help of molecular dynamic simulation. The large value of the pre-exponential factor should be noted, which requires further detailed investigations.

1. Introduction
There is a phenomenon of fracture in tensile stresses, which takes place, for example, during the interaction of a plane shock wave with a flat rear surface [1, 2] or interaction of unloading waves generated by reflection of a cylindrical diverging shock wave from the flat faces [3]. During the process large transient tensile stresses appear which lead to the fracture of the material. Such a specific type of dynamic fracture, caused by the interaction of unloading waves is known as spalling [1, 4, 5]. The basic example of such a phenomenon is a reflection of a plane shock wave on the sample’s free flat surface. Such shock wave can be caused by imploding a charge or using a high-speed blow plate that forms up a flat shock wave at the surface of the sample. This phenomenon is described by various failure models, in particular the multi-scale model [6, 7]. The model includes equations, in particular the equation for the speed of the formation of a homogeneous cavities, which in turn need more verification. Homogeneous formation of cavities, melting and crystallization centers was investigated in [6–10] by molecular-dynamic calculations with the construction of multi-scale models. The rate of a homogeneous nucleation of nanovoids in expanded aluminum is researched in this work by using the method proposed in [6–10].

2. Results and discussion
The formation of pores in the solid aluminum in the stretched state under action of negative pressure is researched by using the method of molecular dynamics (MD). The time of the sample life at a temperature of 300 and 500 K for targets subjected to several pressure levels for each temperature is determined during the experiment. Statistical straggling is taken into account by several simulations of MD trajectories for each of the target temperature and pressure. The calculations are performed by LAMMPS package [11]; EAM potential of interatomic interactions AL99 is used [12]. The sample contains 256 000 aluminum atoms formed in a cubic shape as the system with fcc lattice. Constant temperature of MD system (300 or 500 K) is permanently kept by a thermostat. Negative pressure is permanently maintained by a barostat with a steady
Figure 1. MD system at the initial moment (aluminum, fcc lattice). Color corresponds to the value of the centro-symmetry parameter illustrating the lattice disordering.

Figure 2. MD system at the time 195 ps: (a) all atoms, (b) selected atoms. Color corresponds to the value of the centro-symmetry parameter illustrating the lattice disordering.

Figure 3. MD system at the time 300 ps: (a) all atoms, (b) selected atoms. Color corresponds to the value of the centro-symmetry parameter illustrating the lattice disordering.
Figure 4. Pressure in MD system versus time for several MD trajectories at temperature 500 K.

Figure 5. The graph of systems number dependence on the life-time for temperatures (a) 300 K and (b) 500 K.

target pressure. Step of time integration is 1 fs, the system is traced prior to the moment of fracture begins. Twenty trajectories are simulated for each pair temperature-pressure of sample; various trajectories are set by varying the initial distribution of velocities of atoms.

The MD sample is shown at successive times in figures 1–3. By the time the system has lived 195 ps, defective atoms appear. These atoms form up the nucleus of void. By the time the system has lived 300 ps, one of the nucleus normally grows into the void. The following growth of the void does not occur as the system is energetically unfavorable to increase the free surface
due to increased surface energy. At the same time a negative pressure in the system decreases to a certain amount that depends on the initial level of impact and trajectory of the system (figure 4).

Figure 5 collects the obtained results for the lifetime of MD systems. X-axis corresponds the time, Y-axis represents the number of systems being in the meta-stable stretched state (without voids) under negative target pressure during this time. This graph is obtained by carrying out a series of calculations at different pressures and trajectories for temperatures 300 and 500 K. The life-time of the system under negative pressure is determined depending on the number of systems in a metastable state (figure 5). Average lifetime is obtained by using exponential approximation for system lifetime

\[ n = n_0 \exp \left( -\frac{\tau}{\langle \tau \rangle} \right), \tag{1} \]

where \( n \)—number of systems in metastable state for current time \( \tau \), \( n_0 \)—initial number of MD trajectories, \( \langle \tau \rangle \)—average lifetime of the system in an expanded state. This method of determination of characteristic lifetime is taken from the works [13, 14].

The characteristic lifetime of systems in metastable state can be used for determination of the rate of void nucleus formation. The nucleation rate \( J \) for various pressures temperatures is calculated according to the following formula taken from [14]

\[ J = \frac{1}{N \langle \tau \rangle}, \tag{2} \]

where \( N \)—number of atoms in the system. The resulting dependencies of the nucleation rate on the pressure are shown in figure 6.

Based on the concepts of thermal fluctuations, the nucleation rate in a homogeneous metal can be written as:

\[ J = J_0 \exp \left( -\frac{16\pi \sigma^2}{3kT P^2} \right), \tag{3} \]
where $T$—temperature, $P$—pressure, $\sigma$—surface tension, $J_0$—pre-exponential factor. The comparison of data obtained with formula (3) with the MD results is shown in figures 6 and 7. From figures 7a, 7b we determine the coefficients for the temperature of 300 K: $J_0 = 1.9 \times 10^8$ ps$^{-1}$, $\sigma = 0.9$ J/m$^2$; and for temperature 500 K: $J_0 = 1.1 \times 10^{12}$ ps$^{-1}$, $\sigma = 1.0$ J/m$^2$.

3. Conclusions

Typical lifetime of the system in a meta-stable state at a negative pressure as well as coefficients of surface tension $\sigma$ and pre-exponential factor of nucleation rate $J_0$ at the temperatures 300 and 500 K are obtained with the help of molecular—dynamic simulation (300 K: $J_0 = 1.9 \times 10^8$ ps$^{-1}$, $\sigma = 0.9$ J/m$^2$; and 500 K: $J_0 = 1.1 \times 10^{12}$ ps$^{-1}$, $\sigma = 1.0$ J/m$^2$). The large value of the pre-exponential factor should be noted, which requires further detailed investigations. Defective areas (cavities embryos) are formed over time in the expended material, with one of the embryos normally growing into the cavity. Further growth of the cavity under pressure does not occur as the system is energetically unfavorable to increase the free surface due to increased surface energy. At the same time a negative pressure in the system decreases to a certain value depending on the initial level of impact and trajectory of the system.

The results obtained in the course of the work, perfectly complement article [15] since we performed calculations for 300 and 500 K temperatures for large volume system of 256 000 atom but with the same potential for interaction [12] and a similar molecular model.

The resulting surface tension coefficient values lie between the values obtained for the melt in the article [16] (0.87–1.03 J/m$^2$) and for solid state at a temperature of 453 K in the book [17] (1.14 J/m$^2$).

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