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TWO LEVEL INVESTIGATION OF PLASTICITY DRIVEN GROWTH OF NANOVOIDS UNDER HIGH RATE TENSION OF ALUMINUM

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Abstract. With the help of molecular dynamics simulations the mechanism of nanovoid growth in aluminum under high rate tension is studied. We interpret the growth of nanovoids as the result of plastic deformation in zone close to void and corresponding atom rearrangement on void surface. The dependencies of critical negative pressure in systems of various atom number and void diameter at various temperatures are researched. It is shown, that critical pressure depends both on void diameter and simulated area size. Increase of temperature leads to linear decrease of system tensile strength. Also, some attention is given to the influence of initial stacking faults on critical pressure. The continuum model connects the void growth rate with the plastic flow around a void. The generation of dislocations near a void surface is described with the Arrhenius type relation; the parameters of this relation are fitted by comparison with molecular dynamics data.

1 INTRODUCTION

Fracture of metals under dynamical loading attracts substantial attention of researchers through last decades [1,2]. Progress in experimental techniques allows today to research the behavior of targets subjected to ultimate high strain rate up to 10^{10} s^{-1} [3]. The data collected in such experiments stimulate the theoretical works in the field of dynamical response of targets.

Fracture and plasticity are coupled processes, that was clearly demonstrated in experiments [4,5] and molecular dynamics (MD) works [6-11]. The basic mechanism of void growth in the conditions of high rate strain as it follows from above cited MD papers is the emission of dislocations from a void surface, the ends of which remain attached to a void providing thereby displacements of surface atoms.

Today the continuum models of fracture under high rate tension [12-17] typically take into account the nucleation of voids, the plasticity, for example, through the plastic potential offered by Gurson [18], and the inertia effect. The additional time scale for fracture is given

from the sensitivity of shear strength of material on the deformation rate [13,14]. Mayer and Krasnikov [15] and Wilkerson and Ramesh [16] offered the models including the plastic relaxation of shear stress in process of fracture through the equations of dislocation motion and kinetics. The authors showed that motion and multiplication of dislocations are important under the high rate tension.

In this paper, we investigate the first stage of fracture in aluminum under high rate tension with the help of MD simulations. We examine an ideal lattice, a lattice with an initial void and a prestrained material. We propose a continuum model of dislocation-based growth of nanovoids in aluminum in order to predict the critical tensile pressure in the deformed region. The main advantage of the offered approach in comparison with works [15,16] is the accounting of dislocation generation near a void surface. This process observed at the MD stage is described with an Arrhenius-type relation for the rate of dislocation nucleation; the parameters of this relation are defined in comparison with obtained MD data.

2 MD SIMULATIONS

The investigation of the initial stage of fracture in aluminum is performed with the parallel MD code LAMMPS [19] with EAM potential [20].

Simulated area represents a cube with side d varying in range from 12 nm to 81 nm, which corresponds to atom number from 108 000 to 32 000 000. Periodic boundary conditions are set for all cube faces. A spherical void is created in the centre of modeled area. The material around the void is an ideal monocrystal. The axes of coordinate system are oriented along (100), (010) and (001) crystallographic directions. The tension is applied along Ox-axis with constant rate of 10^8, 10^9 or 10^{10} s^{-1}. The simulations are performed at 100, 300, 600 and 900 K; the system temperature is kept constant with nvt-thermostat during deformation. Before straining the system is relaxed at atmospheric pressure and fixed temperature over 2 ps with lattice parameter a=0.405 nm. When we consider a region with initial dislocations, we deform the region by pure shearing to 0.125 strain in order to create a dislocation structure in the material. The cycle of shearing includes a straight and reverse shift of the region's upper boundary so that the initial form is restored after this procedure. The additional relaxation is run during 10 ps after the cycle of shearing.

A defect structure is analyzed with the centro-symmetry parameter [21]. Atomic configurations are visualized with the OVITO tool [22]. The free volume is calculated with the help of a utility, which divides the simulated region into small identical cubes with the side length equal to the initial lattice parameter. If there are no atoms in the fixed small cube, the volume of the cube is added to the total void volume.

2.1 Tension of region with perfect lattice

Homogeneous generation of dislocations occurs after reaching the critical shear stress in the region without any initial defects. Generation of dislocations starts from the formation of a high enough concentration of uniformly distributed nuclei, which are shaped like the ellipsoids elongated in the direction of 45° to the Ox- and Oy-axes of the system. The nuclei lying in the same slip plane consolidate into a thin stacking fault plane bounded by dislocation lines. The generation of dislocations by this mechanism occurs in all the calculations performed; at the same time, a tendency to a decrease in the uniformity of stacking fault plane

distribution is observed together with a drop in the strain rate from 10^{10} to 10^{8} s^{-1}. In paper [23] it was reported about a similar mechanism of homogeneous generation of dislocations under simple shear. Generation and subsequent motion of dislocations lead to effective relaxation of shear stress in the simulated region; this process is depicted in figure 1 for deviatoric stress. A further growth of the deformation degree leads to the nucleation of voids, the size of which grows starting from the interatomic distance. The void nuclei arise mainly at the intersections of the stacking fault planes. Appearance of voids leads to a system stability loss, and, consequently, the pressure in the region sharply decreases in magnitude.

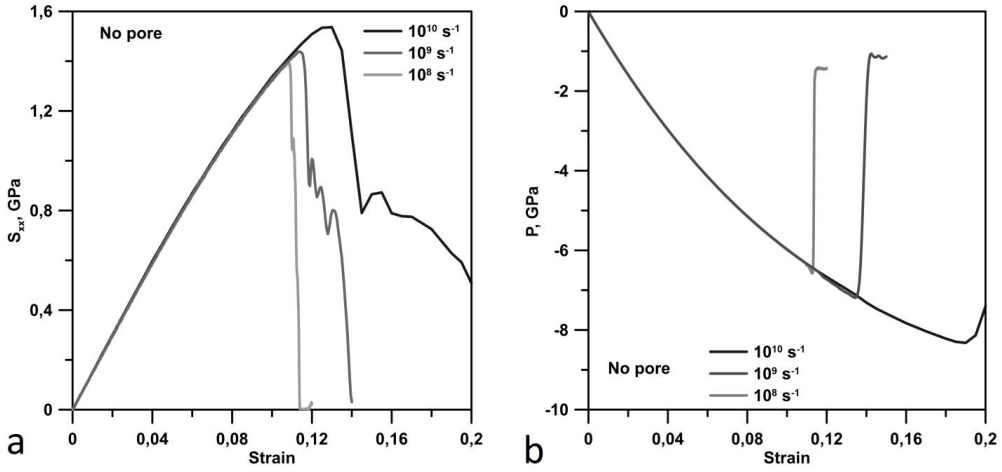

Figure 1: (a)-deviatoric stress, (b)-pressure in region versus strain. Various strain rates. The system size is d = 16.2 nm.

2.2 Tension of region with initial void

Plastic relaxation leading to a drop in the shear stress in the region is activated together with the beginning of the void growth (see figure 2). The critical deviatoric stress is a weak function of the size of the simulated region if the initial radius of the void is fixed (figure 2a); it slightly rises together with increase in the region size. Therefore, the start time of the plastic growth of the void is practically the same for systems of various sizes containing identical initial voids (figure 2c). The critical deviatoric stress is very sensitive to the initial void radius at a constant void size (figure 2b), the increase in the void radius leads to a decrease in the threshold deviatoric stress and, consequently, earlier beginning of the void growth (figure 2d).

Figures 2c and 2d demonstrate that the increase in the ratio of the initial void radius to the system size induces a tendency to postpone the critical pressure achievement after the start of the plastic growth of the void and, as a result, leads to a higher absolute value of pressure in the system. It is demonstrated that the threshold pressure depends both on the initial void radius and on the system size.

The mechanism of the initial void growth consists of the dislocation emission from the void surface and corresponding addition of some extra volume to the void volume; the appearance of this extra volume is associated with the motion of the dislocation half-plane edge into the material. Further development of plastic deformation leads to the formation of a zone with an active plastic flow around the void; this zone is characterized by a large number

of dislocations. The displacement of atoms occurs over the entire void surface, but the atoms lying near the first emitted dislocations acquire the maximum displacement. Therefore, the growth of the void is enabled by the rearrangement of atoms on and near the surface, which is the consequence of the plastic flow development in the surrounding zone with a higher dislocation density.

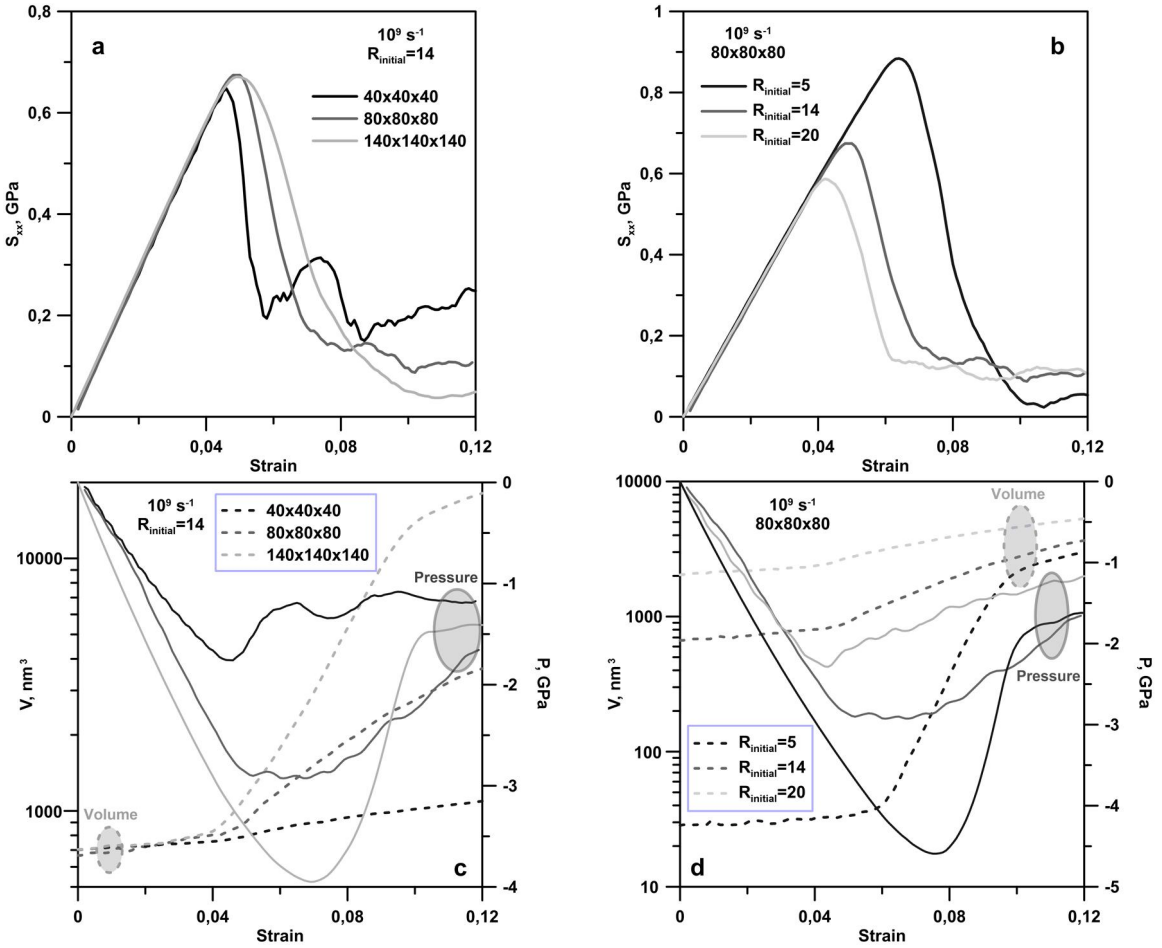

Figure 2: Deviatoric stress (a, b), void volume and pressure (c, d) in the system as a function of strain. (a), (c)-radius of initial void is R_{in}= 5.67 nm, various system sizes; (b), (d)-system size d = 32.4 nm, various radii of initial void. The system sizes and the void radii are given in the figures on the scale of the deformation-free lattice constant (a = 0.405 nm); the strain rate is 10^9 s^{-1}.

The temperature dependence of the critical pressure in the system is studied in order to check the thermoactivated nature of the void growth initiation. It is shown that the decrease in the tensile strength of aluminum with a nanovoid while heating can be approximated with high accuracy by a linear law (see figure 4b). Also, the tensile strength increases substantially together with the rise in the strain rate. Therefore, we suppose that the formation of dislocations at the void surface is a thermoactivated process and we use an Arrhenius-type relation to take into account the rate of dislocation nucleation in section 3, just as in papers [11,23].

2.3 Tension of the region with initial dislocations

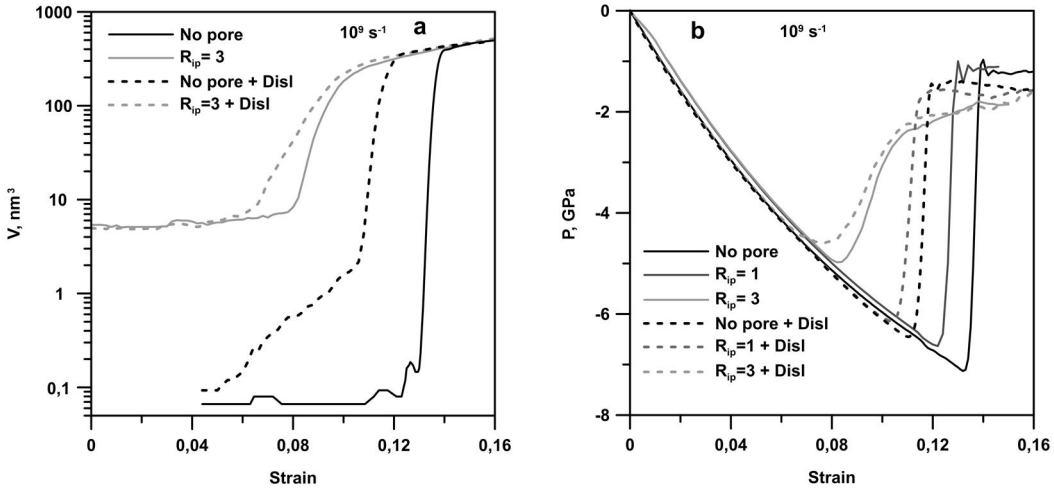

Figure 3: (a)-free volume in various systems (ideal lattice with or without initial void, prestrained material with or without initial void), (b)-pressure in the region versus strain. The strain rate is 10^9 s^{-1}. System size is d = 16.2 nm.

After the process of initial dislocation creation, the structure of the material contains stacking fault planes, vacancies and clusters of vacancies. When tension is applied to the region, both the formation of dislocations from vacancy clusters and the slipping of initially existing dislocations are observed. If the target has no initial voids, secondary voids appear at the intersections of the stacking fault planes or in the preexisting vacancy clusters, because the lattice there has the highest concentration of defects. The nucleation and growth of secondary voids include two stages: 1) at the first stage, the number of the void nucleation centers increases, which manifests itself in a gradual growth of the free volume in the deformed region, 2) at the second stage, the volume of nucleated voids rapidly grows without formation of new voids (the evolution of free volume is presented in figure 3a). If there is a pre-existing initial void in the region, the initial dislocation loops begin to grow towards the void surface, and, as a result, the void volume begins to increase earlier compared to the case of ideal lattice. Critical pressures are lower in the case of prestrained region compared to the ideal lattice (figure 3b), because the lattice is initially weakened and plastic relaxation starts earlier.

3 CONTINUUM MODEL

3.1 Model formulation

As it is demonstrated in section 2.2, nanovoids grow through plastic deformation around the void. We assume that volume change of void is entirely defined by plastic deformations in zone, where shear stress exceeds static yield strength of material $\sigma_\tau \geq Y/2$. The radius of this zone can be estimated using the solution of equilibrium equation in the case of spherical symmetry [24] as follow

$$r_{\text{pl}} = R \cdot \left[2\sigma_\tau^{\max} / Y \right]^{1/3} \tag{1}$$

where $\sigma_\tau^{\max} = (3/4)(-P - 2\gamma / R)$, R is the radius of initial void, P is the pressure infinitely far from the void, γ is the surface tension coefficient. In the first approximation the change of void radius is obtained taking into account the effective plastic strain w in this zone

$$\dot{R} = \dot{w} \cdot (r_{\text{pl}} - R). \tag{2}$$

Plastic deformation rate $\dot{w}$ can be found from the Orowan equation [25], which is written in the simplest form

$$\dot{w} = \frac{b}{\sqrt{6}} V_{\text{D}} \cdot \rho_{\text{D}}, \tag{3}$$

where b is the module of Burger's vector, V_{D} is the dislocation velocity, ρ_D is the scalar density of dislocations. In this work we use a simple stationary form of the equation of dislocation motion

$$BV_{\text{D}} = b\left[\sigma_\tau^{\max} - Y/2\right] \cdot \left[1 - (V_{\text{D}} / c_{\text{t}})^2\right]^{3/2}, \tag{4}$$

B is the phonon friction coefficient increasing with the temperature rise [26], $c_{\text{t}} = G/\rho$ is transverse sound velocity, G is the shear modulus, ρ is the material density.

As follows from the MD results the nucleation of dislocations near void surface plays the key role in process of void growth. According with this fact we consider two mechanisms of the dislocation density increase: nucleation of dislocations and dislocation multiplication. We take into account the nucleation of dislocations in zone close to void through Arhenius-type relation analogically with [11,23] and introduce the following equation of the dislocation density balance

$$\frac{d\rho_{\text{D}}}{dt} = 2\pi c_t N \cdot \exp\left(-\frac{U - V_0 \cdot \sigma_\tau^{\max}}{kT}\right) + \frac{0.1}{\varepsilon_{\text{D}}}\left(b \cdot \sigma_\tau^{\max} \cdot V_{\text{D}}\right)\rho_{\text{D}}. \tag{5}$$

The first term considers the nucleation of dislocations near the void surface, the multiplier before exponent is a product of nucleation centers number per unit volume (which is defined by concentration of the voids in the substance N) by the length of dislocation segment $2\pi R$ arising in one nucleation act and by the characteristic frequency, which can be estimated as c_{t} / R. In exponent power U is the nucleation energy, V_0 is the activation volume. The second term allows for the dislocation multiplication and it is taken from our previous works [27,28], $\varepsilon_{\text{D}} = 8\,\text{eV}/b$ is the dislocation formation energy per unit length.

3.2 Modeling results

The modeling of nanovoid growth in aluminum under high rate tension is carried out with the help of system of Eqs. (1)-(5). The volume of the modeled area V is increased with the constant deformation rate $\dot{\varepsilon}$. The temperature of the substance remains constant as well as it behaves in MD study. The pressure is found through wide range equation of state offered in [29].

When the pressure reaches a certain value, which depends on the temperature, the strain rate, the void radius and the distance between their centers (since concentration), the plastic flow starts and the void radius grows irreversible. But pressure in the system continues to drop until the rate of the void growth does not equalize with the rate of the system volume

increase. In this moment the maximal magnitude of pressure is reached; this is the point of dynamical tensile strength of aluminum with initial voids.

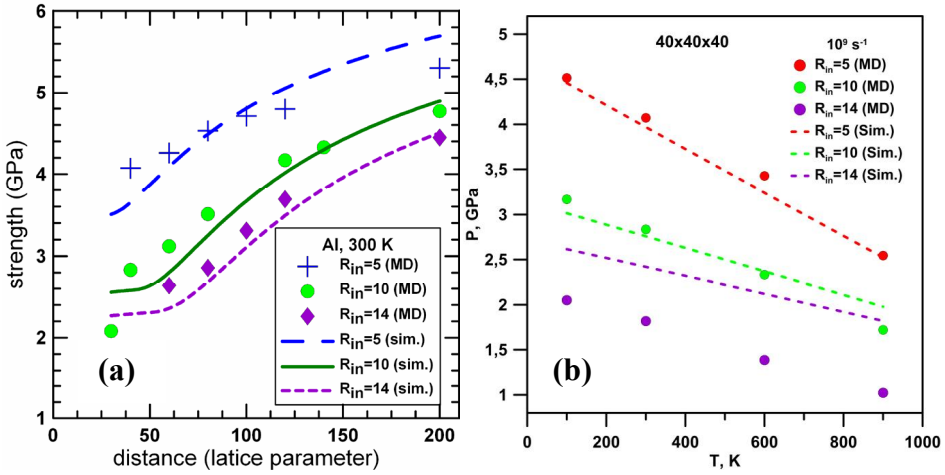

Figure 5. Results of continual modeling by dislocation model (lines) in comparison with MD data (points): (a) - dependence of tensile strength on distance between centers of voids; (b) - dependence of tensile strength on temperature T. Radii of initial void are given in scale of the undeformed lattice constant (a=0.405 nm). Strain rate is 10^9 s^{-1}.

Fig. 5 demonstrates the continual results on critical pressure obtained with above stated model in comparison with MD results. From the data presented in Fig. 5 it follows that the dislocation model qualitatively correctly describes the behavior of the system depending on the radius, the distance between the voids (the size of the system in MD simulations) and the temperature. The quantitative agreement is obtained with the following model parameters: $U = 3.1\,\text{eV}$, $V_0 = 0.5\,\text{nm}^3$ and $\gamma(T) = \left(2.67 - T \cdot 0.002\,\text{K}^{-1}\right)\text{J/m}^2$; the values of the other parameters are taken from the works [27,28]. The determined value of the activation volume closes to that given in [23] for the case of homogeneous nucleation of dislocations in a perfect crystal. Obtained energy of nucleation is 1.5-2 times lower than the value determined in [23], but it is expected, since in our case the dislocation nucleation occurs near the voids, which should significantly reduce the energy barrier.

4 CONCLUSIONS

We studied the initial stage of fracture occurring in the materials with different initial structure: ideal lattice with or without void, material containing initial dislocations and vacancies with or without void. In all cases the activation of plastic relaxation precedes the void nucleation and growth. The nucleation of voids occurs in intersections of stacking faults planes or vacancies clusters. The mechanism of void growth is formation or slipping of preexisting dislocations and further plastic flow around the void and corresponding rearrangement of atoms on the entire void surface. These facts mean that continual modeling of fracture is directly connected with description of plastic flow.

The dislocation based continual model of nanovoid growth is offered to describe the plastic flow near a void and the related void growth. Generation of dislocations near a void surface in

substance is taken into account with Arrhenius-type relation for nucleation rate of dislocations. Fitted value of activation volume is close to the case of homogeneous dislocation formation in pure aluminum and the nucleation energy is lower than the value reported in the work [23].

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