Initial stage of fracture of aluminum with ideal and defect lattice

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Abstract. In this work, we investigate the initiation of fracture in an aluminum sample with the help of molecular dynamics simulations. The critical negative pressures in different simulated regions as a function of the system size and initial structure are obtained. Tension in regions with defect structures, such as initial voids or dislocations and vacancies, leads to a decrease in tensile strength. In case of initial voids, a decrease in the ratio of the void radius to the system size causes an increase in the system’s tensile strength, while rising temperature causes a linear drop of tensile strength. We propose a continuum dislocation based model of nanovoids growth to describe the critical negative pressure in systems with a void. Nucleation of dislocations near a growing void is taken into account with the Arrhenius-type law for the nucleation rate.

1. Introduction
Fracture of metals under dynamical loading attracts substantial attention of researchers through last decades [1–3]. Progress in experimental techniques allows today to research the behavior of metals subjected to ultimate high strain rate up to $10^{10}$ s$^{-1}$ [4, 5]. The data collected in such experiments stimulate the theoretical works in the field of dynamical response of targets. The accurate description of matter dynamics requires the knowledge of equation of state [6] and the accounting of the rate and temperature dependent plastic relaxation and fracture models. Usage of the multiscale approach, when the continuum model is based on the atomistic simulations, looks promising for modeling of high rate deformations.

Fracture and plasticity are coupled processes, and this was clearly demonstrated in many experiments [7–9]. The fracture and corresponding plastic flow under high rate tension were extensively studied in many molecular dynamic (MD) works [10–25]. Some of these works were devoted to simulation of nucleation and growth of voids in initially perfect crystal [10–12, 16, 21]; the authors of other papers examined more detailed the mechanisms of initially existing void growth [13–15, 18–21, 23–25]; in [22] the nucleation and growth of voids in the crystal with defect structure arisen during the anterior shock passage were investigated. The basic mechanism of void growth in the conditions of high rate strain as it follows from above cited papers is the emission of dislocations from void surface, the ends of which remain attached to a void providing thereby displacements of surface atoms. The authors of [15, 21] demonstrated that an increase of temperature up to the melting point provokes the change of void growth mechanism in aluminum from the dislocation generation to viscous-like type, when the material around a void can be considered as melted one. On the basis of the nucleation and growth approach [26], a fracture
model of aluminum was proposed in [15, 21] that use a very simplified equation of the void growth.

Today the continuum models of fracture under high rate tension [27–36] typically take into account the nucleation of voids, the plasticity, for example, through the plastic potential offered by Gurson [37], and the inertia effect. The inertial effect associated with the accelerated motion of material close to a void becomes the significant role in the case of a high rate deformation as it was stated in [28, 29]. The additional time scale for fracture is given from the sensitivity of shear strength of material on the deformation rate [29, 33]. Mayer and Krasnikov [34] offered the model dealing with plastic relaxation of shear stress around a crack through the equations of dislocation motion and kinetics. It was stated that the influence of dislocation dynamics and kinetics on crack growth depends both on the crack size and deformation rate. Wilkerson and Ramesh [36] formulated the model containing the equations of dislocation motion and kinetics. The authors showed that motion and multiplication of dislocations are more important in comparison with inertia effect for nanovoid growth under 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 [34, 36] 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. Molecular dynamics simulations

2.1. MD setup

The investigation of the initial stage of fracture in aluminum is performed with the parallel MD code LAMMPS [38] with EAM potential [39].

The simulated region represents a cube with a side length $d$ varying from 12 nm to 81 nm, corresponding to 108,000 to 32,000,000 atoms. The periodic boundary conditions are set for all the cube faces. 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. A spherical void is created in the center of the simulated region by means of the LAMMPS standard “delete atoms” command. The axes of the coordinate system are oriented along the (100), (010) and (001) crystallographic directions. In all cases, tension is applied along the $Ox$-axis at a constant rate of $10^8$, $10^9$ or $10^{10}$ s$^{-1}$. Such loading conditions agree with the case of a planar shock wave reflection on the back surface, when lateral release is negligible. The system temperature is kept constant with the help of the “nvt” thermostat during tension. Before deformation, the system is relaxed at atmospheric pressure and fixed temperature for 2 ps with a lattice parameter of $a = 0.405$ nm in the case of the void-bearing material, with additional 10-ps relaxation after the cycle of shearing.

A defect structure is analyzed with the centro-symmetry parameter [40]. Atomic configurations are visualized with the OVITO tool [41]. 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.

2.2. Tension of region with perfect lattice

Homogeneous generation of dislocations occurs after reaching the critical shear stress in the region without any initial defects (figure 1). Generation of dislocations starts from the formation
Figure 1. Formation of dislocations and voids in the ideal lattice under tension at a strain rate of $10^9$ s$^{-1}$. The system size is $d = 16.2$ nm. Only atoms with locally defective environment are shown. Time in picoseconds is given in the upper left corner.

of a high enough concentration of uniformly distributed nuclei, which are shaped like the ellipsoids elongated in the direction of $45^\circ$ 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 [42] 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 2 for deviatoric stress. The critical
deviatoric stress corresponding to the strain rate of $10^8$, $10^9$ and $10^{10}$ s$^{-1}$ is 1.39, 1.44 and 1.54 GPa (figure 2). A further growth of the degree of deformation leads to the nucleation of voids, the size of which grows starting from the interatomic distance (figure 1 135 and 139 ps). 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 2). The maximal absolute value of negative pressure is the dynamic tensile strength of perfect monocrystal that is equal to 6.5, 7.1 and 8.4 GPa for strain rates of $10^8$, $10^9$ and $10^{10}$ s$^{-1}$ respectively. These values do not contradict to an estimation 5.8–6.4 GPa of the tensile strength of aluminum for the strain rate of $10^9$ s$^{-1}$ that were experimentally obtained at ultra-short laser irradiation of thin aluminum films [4], as well as to MD simulation results [22, 43].

2.3. Tension of the 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 3). 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 3a); 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 3c). The critical deviatoric stress is very sensitive to the initial void radius at a constant void size (figure 3b), the increase in the void radius leads to a decrease in the threshold deviatoric stress and, consequently, earlier beginning of the void growth (figure 3d).

Figures 3c and 3d demonstrate that the decrease 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
Figure 3. 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 $R_{\text{initial}} = 5.67$ 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$^{-1}$.

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.

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
Figure 4. (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 $10^9 \text{s}^{-1}$. System size is $d = 16.2$ nm.

accuracy by a linear law (see figure 5). 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 [25, 42].

2.4. Tension of the region with initial dislocations
After the process of initial dislocation development presented in section 2.1, the structure of the material contains stacking fault planes bounded by dislocation loops, 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 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 4a). 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 4b), because the lattice is initially weakened and plastic relaxation starts earlier.

3. Continuum model
3.1. Model formulation
As demonstrated in section 2.3, nanovoids grow through plastic deformation around the void. We assume that the change in the void volume is completely controlled by plastic deformations
in the zone, where the shear stress exceeds the static yield strength of the material \( \sigma \geq Y/2 \).

The radius of this zone can be estimated by solving the equilibrium equation in the case of spherical symmetry [44] as follows:

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

(1)

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

\[
\dot{R} = \dot{w} (r_{pl} - R).
\]

(2)

Plastic strain rate \( \dot{w} \) can be found from the Orowan equation [45], which is written in the simplest form:

\[
\dot{w} = \frac{b}{\sqrt{6}} V_D \rho_D,
\]

(3)

where \( b \) is the Burgers vector magnitude, \( V_D \) is the dislocation velocity, \( \rho_D \) is the scalar density of dislocations. In this work we use a simple stationary form of the equation of dislocation motion:

\[
BV_D = b \left[ \sigma_{\text{max}}^\tau - Y / 2 \right] \left[ 1 - \left( V_D / c_l \right)^2 \right]^{3/2},
\]

(4)

where \( B \) is the phonon friction coefficient growing with temperature [46], \( c_l = G / \rho \) is the transverse sound velocity, \( G \) is the shear modulus, \( \rho \) is the material density.

As follows from the MD results, the nucleation of dislocations near void surface plays the key role in the process of void growth. In accordance with this fact, we consider two mechanisms of the dislocation density growth: nucleation of dislocations and multiplication of dislocations. We take into account the nucleation of dislocations in the zone close to the void through the Arrhenius-type relation by analogy with [25, 42] and introduce the following equation of dislocation density balance:

\[
\frac{d\rho_D}{dt} = 2\pi c_l N \exp \left( \frac{-U - V_0 \sigma_{\text{max}}^\tau}{kT} \right) + 0.1 \frac{1}{\varepsilon_D} \left( b \sigma_{\text{max}}^\tau V_D \right) \rho_D.
\]

(5)

The first term considers the nucleation of dislocations near the void surface, the multiplier before the exponent is a product of the number of nucleation centers per unit volume (which is determined by the concentration of voids in the substance \( N = d^{-3} \)) by the length of the dislocation segment \( 2\pi R \) arising in one nucleation act and by the characteristic frequency, which can be estimated as \( c_l / R \). In the 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 [47, 48], \( \varepsilon_D = 8 \text{ eV} / b \) is the dislocation formation energy per unit length.

3.2. Results of continuum modeling

Modeling of the nanovoid growth in aluminum under high rate tension is carried out with the help of the system of equations (1)–(5). The volume of the simulated region \( V \) is increased at a constant strain rate \( \dot{\varepsilon} \). The temperature of the substance remains constant similarly to the MD study. The pressure is calculated by the wide-range equation of state proposed in [49].

When the pressure reaches a certain value, which depends on temperature, strain rate, void radius and distance between their centers (i.e. concentration), a plastic flow occurs and the void radius grows irreversibly. However, pressure in the system continues to drop until the rate of the void growth does not equalize with the rate of the system volume growth. At this moment,
Figure 5. Results of continuum modeling by the dislocation model (lines) in comparison with MD data (points): (a)—tensile strength as a function of distance between void centers; (b)—tensile strength as a function of temperature $T$. Radii of initial voids are given on scale of the deformation-free lattice constant ($a = 0.405$ nm). The strain rate is $10^9$ s$^{-1}$.

The maximum magnitude of pressure is reached; this is the point of dynamic tensile strength of aluminum with initial voids.

Figure 5 demonstrates the continuum modeling results for critical pressure obtained by the above stated model in comparison with MD results. From the data presented in figure 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: $U = 3.1$ eV, $V_0 = 0.5$ nm$^3$ and $\gamma(T) = (2.67 - T \times 0.002$ K$^{-1})$ J/m$^2$: the values of the other parameters are taken from [47,48]. The calculated value of the activation volume is close to that given in [42] for the case of homogeneous nucleation of dislocations in a perfect crystal. The calculated energy of nucleation is 1.5–2 times lower than the value obtained in [42], but this could be expected, since in our case dislocations occur near voids, which should significantly reduce the energy barrier.

4. Conclusions

We studied the initial stage of fracture occurring in the materials with different initial structures: ideal lattice with or without void, material containing initial dislocations and vacancies with or without void. In all the cases, the activation of plastic relaxation precedes the void nucleation and growth. The nucleation of voids occurs at intersections of stacking fault planes or vacancy clusters. The mechanism of void growth consists in the 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 continuum modeling of fracture is directly connected with the description of plastic flow.

The dislocation based continuum model of nanovoid growth is proposed to describe the plastic flow near a void and the related void growth. This model is a development of approach to
fracture description with direct solving of equations for defects dynamics and kinetics offered in works [34,36]. Generation of dislocations near a void surface in a substance is taken into account with an Arrhenius-type relation for the nucleation rate of dislocations. The fitted value of the 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 [42].

Further development of the framework proposed in this paper consists in the accounting for the homogeneous nucleation of dislocations in the ideal lattice and for the nucleation of voids in weakened zones of the crystal. Together with the proposed model of void growth, the equations for void nucleation rate will form a full model that should be applicable for description of laser experiments with thin metal foils, for example [4, 5], as well as impact experiments, for instance [2,3].

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References
[1] Staudhammer K P, Murr L E and Meyers M A 2001 *Fundamental Issues and Applications of Shock-Wave and High Strain-Rate Phenomena* (Oxford: Elsevier)
[2] Zaretsky E B and Kanel G I 2012 *J. Appl. Phys.* **112** 073504
[3] Kanel G I, Razorenov S V, Garkushin G V, Ashitkov S I, Komarov P S and Agranat M B 2014 *Phys. Solid State* **56** 1569–1573
[4] Ashitkov S I, Agranat M B, Kanel G I, Komarov P S and Fortov V E 2010 *JETP Lett.* **92** 516–520
[5] Ashitkov S I, Komarov P S, Agranat M B, Kanel G I and Fortov V E 2013 *JETP Lett.* **98** 384–388
[6] Khishchenko K V 2015 *J. Phys.: Conf. Series* This issue (Preprint arXiv:1510.00763)
[7] Rice J R and Thomson R 1974 *Philos. Mag.* **29** 73–96
[8] Christy S 1986 *Metallurgical Applications of Shock-Wave and High-Strain-Rate Phenomena* (New York: Dekker)
[9] Meyers M A 1994 *Dynamic Behavior of Materials* (New York: Wiley-Interscience)
[10] Lynden-Bell R M 1995 *J. Phys.: Condens. Matter* **7** 4603
[11] Belak J F 1998 *Comput. Aided Mater. Des.* **5** 193
[12] Rudd R E and Belak J F 2002 *Comput. Mater. Sci.* **24** 148
[13] Seppala E T, Belak J F and Rudd R E 2005 *Phys. Rev. B* **71** 064112
[14] Ahn D C, Sofronis P, Kumar M, Belak J and Minich R 2007 *J. Appl. Phys.* **101** 063514
[15] Kuksin A Y and Yanilkin A V 2007 *Dokl. Phys.* **52** 186–190
[16] Norman G E, Stegailov V V and Yanilkin A V 2007 *High Temp.* **56** 164–172
[17] Kuksin A Y, Stegailov V V and Yanilkin A V 2008 *Phys. Solid State* **50** 1984–1990
[18] Traiviratana S, Bringga E M, Benson D J and Meyers M A 2008 *Acta Mater.* **56** 3874–3886
[19] Rudd R E 2009 *Philos. Mag.* **89** 3133–3161
[20] Bringga E M, Traiviratana S and Meyers M A 2010 *Acta Mater.* **58** 4458–4477
[21] Kuksin A Y, Norman G E, Stegailov V V, Yanilkin A V and Zhilyaev P A 2010 *Int. J. Fract.* **162** 127–136
[22] Zhilyaev P A, Kuksin A Y, Stegailov V V and Yanilkin A V 2010 *Phys. Solid State* **52** 1619–1624
[23] Xu S Z, Hao Z M, Su Y Q, Yu Y, Wan Q and Hu W J 2011 *Comput. Mater. Sci.* **50** 2411–2421
[24] Tang Y, Bringga E M and Meyers M A 2012 *Acta Mater.* **60** 4856–4865
[25] Nguyen L D and Warner D H 2012 *Phys. Rev. Let.* **108** 035501
[26] Barbee T W, Seaman J L, Crewdson R J and Curran D R 1972 *J. Appl. Phys.* **43** 393–401
[27] Tvergaard V 1990 *Adv. Appl. Mech.* **27** 83–147
[28] Ortiz M and Molinari A 1992 *J. Appl. Mech.* **59** 48–53
[29] Tong W and Ravichandran G 1995 *J. Appl. Mech.* **62** 633–639
[30] Cuitino A M and Ortiz M 1996 *Acta Mater.* **44** 427–436
[31] Benzeraga A A, Besson J and Pineau A 2004 *Acta Mater.* **52** 4639–4650
[32] Wen J, Huang Y, Hwang K C, Liu C and Li M 2005 *Int. J. Plast.* **21** 381–395
[33] Wright T W and Ramesh K T 2009 *Int. J. Impact Eng.* **36** 1242–1249
[34] Mayer A E and Krasnikov V S 2011 *Eng. Fract. Mech.* **78** 1306–1316
[35] Jacques N, Mercier S and Molinari A 2012 *J. Mech. Phys. Solids* **60** 665–690
[36] Wilkerson J W and Ramesh K T 2014 *J. Mech. Phys. Solids* **70** 262–280
[37] Gurson A L 1977 *J. Engng. Mater. Technol.* **99** 2–15
[38] Plimpton S J 1995 *J. Comp. Phys.* **117** 1–19
[39] Jacobsen K W, Norskov J K and Puska M J 1987 *Phys. Rev. B* **35** 7423–7442
[40] Kelchner C L, Plimpton S J and Hamilton J C 1998 *Phys. Rev. B* **58** 11085
[41] Stukowski A 2010 *Model. Simul. Mater. Sci. Eng.* **18** 015012
[42] Norman G E and Yanilkin A V 2011 *Phys. Solid State* **53** 1614–1619
[43] Zhakhovskii V V, Inogamov N A, Petrov Y V, Ashitkov S I and Nishihara K 2009 *Appl. Surf. Sci.* **53** 9592
[44] Landau L D and Lifshitz E M 1986 *Course of Theoretical Physics. Theory of Elasticity* (New York: Pergamon)
[45] Kosevich A M 1965 *Sov. Phys. Usp.* **7** 837–854
[46] Kuksin A Y and Yanilkin A V 2013 *Phys. Solid State* **55** 931
[47] Krasnikov V S, Mayer A E and Yalovets A P 2011 *Int. J. Plast.* **27** 1294–1308
[48] Mayer A E, Khishchenko K V, Levashov P R and Mayer P N 2013 *J. Appl. Phys.* **113** 193508
[49] Kolgatin S N and Khachatur’yants A V 1982 *Teplofiz. Vys. Temp.* **20** 90–94