Continuum model of tensile fracture of pure aluminum and D16 alloy and its application to the shock wave problems

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Abstract. A continuum model of tensile fracture of solid metals is formulated for the cases of pure aluminum and D16 alloy. It is verified within a wide range of strain rates using results of molecular dynamics simulations and known experimental data. The model considers the growth of spherical voids driven by plastic deformation in their vicinities. Both thermo-fluctuation nucleation of new voids and growth of the pre-existing ones are considered. The stress concentration areas near inclusions are taken into account in the case of alloy. The model is applied to description of the back-side spallation of metal targets exposed to the shock wave loading initiated by high-velocity impact; calculations are performed in 1D case. Results of comparison with known experimental back surface velocity histories are presented.

1. Introduction

Tensile (spall) fracture is a substantial phenomenon, which affects the behavior of materials at the shock loading [1–4]. Metal can fall into a metastable state at negative pressure due to extension in a tension wave formed at reflection of a compression pulse (shock wave followed by unloading wave) from a free surface or release of heated matter in the energy absorption zone of a powerful laser [5–8] or a high-current electron beam [9–12]. Decay of this metastable state is the tensile fracture, which is realized by means of nucleation and growth of voids.

Construction of a fracture model applicable in a wide range of strain rates is an important step for interpretation of the existing experimental data and for using in the mathematical modeling of dynamic processes [13, 14]. Fracture models included in continuum simulations are typically based on various model equations for growth kinetics of some damage parameters. Nucleation and growth method [15] is the most physically based approach because it uses concentrations and sizes of arising voids as natural and measurable damage parameters. Various realizations [16–18] of this method differ by particular equations for concentrations and sizes of voids. A continuum model of tensile fracture is formulated here for pure aluminum and D16 alloy basing on the previously obtained results of molecular dynamics (MD) simulations.

2. Continuum model of fracture

2.1. Continuum mechanics equations and fracture tensor

The fracture model follows the nucleation and growth approach [15] and is based on the equation of plastic growth of spherical voids in metal at tension that was proposed in [19] on the basis
of MD simulations. The influence of voids is taken into account by means of the tensor $W$ of the material deformation at the expense of formation and growth of voids \cite{20}, which we refer as the fracture tensor. Continuum mechanics equations in Lagrange frame of reference have the following form:

\begin{align}
\dot{\rho} &= -\rho \left[ (\nabla \cdot \mathbf{v}) + \dot{W} \right], \\
\dot{\mathbf{v}} &= \frac{1}{\rho} \left[ - (\nabla P) + (\nabla \cdot \mathbf{S}) - P (\nabla W) - (\mathbf{S} \cdot \nabla) W \right], \\
\dot{E} &= \frac{1}{\rho} \left[ -P \left( (\nabla \cdot \mathbf{v}) + \dot{W} \right) + (\mathbf{S} : \mathbf{w}) \right] + D,
\end{align}

where (1) is the equation of continuity, (2) is the equation of motion, (3) is the equation for internal energy; $\rho$ is the substance density; $\mathbf{v}$ is the velocity field; $W = \text{trace} (\mathbf{W})$; $P$ is the pressure; $\mathbf{S}$ is the tensor of stress deviators; $E$ is the specific internal energy; $\mathbf{w}$ is the tensor of plastic deformation; $D$ is the energy absorption function that takes into account the effect of irradiation if any. The pressure is calculated using the wide-range equation of state \cite{21}, which gives one the following dependences

\begin{align*}
P &= P (\rho, E), \\
T &= T (\rho, E),
\end{align*}

where $T$ is the temperature.

The tensor of stress deviators $\mathbf{S}$ and the tensor of plastic deformation $\mathbf{w}$ are calculated using the dislocation plasticity model \cite{14, 22}.

Assuming that all arising voids have a spherical shape, one can obtain that only diagonal components of the tensor $W$ are non-zero, and each of the diagonal components is equal to $W/3$,

\begin{equation}
W = \ln (1 - \alpha).
\end{equation}

Here $\alpha$ is the volume fraction of voids.

2.2. Fracture of pure aluminum

Consider a pure macroscopically uniform metal in the process of tensile fracture. For the sake of simplicity, we suppose that all spherical voids have the same (mean) radius $R$. In this case, the volume fraction of voids $\alpha$ is equal to

\begin{equation}
\alpha = \frac{4\pi}{3} R^3 n,
\end{equation}

where $n$ is the concentration of voids.

According to \cite{19}, the growth rate of void radius $R$ is determined by the plastic deformation by means of the dislocations motion in the void vicinity

\begin{equation}
\left( \dot{R} \right)_p = R \left[ (2\sigma^\text{max}_\tau / Y)^{1/3} - 1 \right] \left( b V_D \rho_D / \sqrt{6} \right),
\end{equation}

where $\sigma^\text{max}_\tau$ is the maximal shear stress arising near the void in the course of its expansion or compression under the action of pressure $P$ and surface tension $\gamma$

\begin{equation}
\sigma^\text{max}_\tau = \frac{G}{K} P - 3G \gamma / R + P (G/K + 1/2) / 2G - \gamma / R,
\end{equation}

where $G$ is the shear modulus, $K = \rho c^2$ is the bulk modulus, $c$ is the sound velocity that is defined by the equation of state; $Y$ is the static yield strength; $b$ is the modulus of Burgers vector; $\rho_D$ is the total scalar density of dislocations within the void vicinity; $V_D$ is the dislocation
velocity in the stress field acting around the void (see equation (7)), which can be found from the following balance equation [19]

\[ V_D = \frac{b}{B} \left[ \sigma^\text{max} - \frac{Y}{2} \right] \left[ 1 - \left( \frac{V_D}{c_t} \right)^2 \right]^{3/2}, \tag{8} \]

where \( B \) is the phonon drag coefficient [23], \( c_t = \sqrt{G/\rho} \) is the transverse sound velocity, which limits the dislocation velocity from above.

The scalar density of dislocations is represented as a sum of two parts \( \rho_D = \rho^a_D + \rho^v_D \), where the first part \( (\rho^a_D) \) is the macroscopic dislocation density, which relates with the macroscopic plastic flow along the spatial scales much larger than the distances between voids. Kinetics of the macroscopic scalar density is determined by the dislocation plasticity model proposed and verified in [14, 22]. The second summand \( (\rho^v_D) \) is an additional dislocation density in the void vicinity that originates from an intensive plastic deformation of the material in the course of voids growth. Dislocation lines formed at this type of plastic flow have complex shapes and curved around the voids [19]; therefore, we suppose that they do not participate in the macroscopic plastic deformation, but only take part in the voids growth. On the contrary, the macroscopic dislocation density takes part in both the macroscopic flow and voids growth. The following kinetics equation is written for \( \rho^v_D \) on the basis of MD simulations [19]

\[ \frac{d\rho^v_D}{dt} = \frac{0.1}{\varepsilon_D} \left( b \sigma^\text{max} V_D \right) \left( \rho^a_D + \rho^v_D \right) - b \rho^v_D (\rho^a_D + \rho^v_D) V_D + \frac{\pi c_t}{2} n \left( \frac{4\pi R^2 b}{a^3_c} \right) \exp \left( -\frac{\pi \varepsilon s a_c}{2k_B T} \right), \tag{9} \]

where the first term in the right-hand part is the generation rate due to the energy dissipation in the course of plastic flow similar to that is used in [14, 22], the second term takes into account the dislocations annihilation [24], and the last term presents the dislocation-loops emission from the void surface [19], which is essential at very high strain rates (about \( 10^8 \text{ s}^{-1} \) and more); \( \varepsilon_s \) is the formation energy of dislocation from void surface per unit length, \( a_c = \varepsilon_s / (b \sigma^\text{max}) \) is the critical radius of the emitted semi-circular dislocation [19], \( \varepsilon_D \) is the energy of dislocation line per unit length, \( k_B \) is the Boltzmann constant. The macroscopic dislocation density is taken into account in equation (9) because according to equation (6) it participates in the plastic flow leading to the void growth. The static yield strength depends on the total dislocation density \( \rho_D = \rho^a_D + \rho^v_D \) in accordance with the Taylor hardening law

\[ Y = Y_0 + 0.5Gb\sqrt{\rho_D}, \tag{10} \]

where \( Y_0 \) is the static yield strength in material with low dislocation density.

Voids can arise in continuous metal due to thermal fluctuations. Analysis of MD data concerning the process of voids nucleation [25–27] shows that the void nuclei arise within the areas of intersection of the stacking fault planes, which can exist initially or be formed in the course of deformation before the fracture beginning. Formation of voids inside the defective areas in solids leads to decrease of the corresponding work, which can be represented as follows

\[ W_c = \frac{16\pi \gamma^3}{3k_B T P^2} \chi, \tag{11} \]

where the dimensionless reduction factor \( \chi \) differs this expression from the case of liquids [20] and takes the lattice defects at the nucleation cites into account. The voids nucleation rate in solids can be written in the same simple form as in liquids [20]

\[ \langle \dot{n} \rangle_1 = \frac{c}{\alpha_4} \exp (-W_c), \tag{12} \]
where $a = \sqrt{\mu / (\rho N_A)}$ is an average interatomic distance, $\mu$ is the molar mass, $N_A$ is Avogadro’s number. The radius of critical voids, which are nucleated and can mechanically grow at the given negative pressure $P$, is equal to

$$R_c = 2\gamma / (-P)$$  \hspace{1cm} (13)$$

where we have taken into account that usually $Y \ll |P|$ at the stage of the active nucleation of voids [28].

In addition to the nucleation, the voids can initially exist in material. Even small initial porosity considerably influences the tensile strength of solids [29,30]. Following [30], we consider an exponential distribution of voids over their surface area. The surface area determines the surface energy of voids and is proportional to the square of its radius. During the tension of material and decreasing the critical radius, more and more new voids from the pre-existing ones become active and begin to grow. It leads to an additional effective source of voids [30]

$$\dot{n} = \frac{2n_0}{\sqrt{\pi} R_0} \exp \left(-\frac{R_c^2}{R_0^2}\right) \left| \frac{dR_c}{dt} \right| \theta \left(\frac{dR_c}{dt}\right)$$  \hspace{1cm} (14)$$

where $\theta(x)$ is the Heaviside function; the critical radius $R_c$ is determined by the current pressure through equation (13); $n_0$ is the total concentration of the initial voids; $R_0$ is the size distribution parameter such that the average radius of the initial voids is equal to $R_0 / (2\pi^{1/2})$.

Combining the nucleation and activation rates, we obtain the total increase rate of the active void concentration

$$\dot{n} = [(\dot{n})_1 + (\dot{n})_2] (1 - \alpha) - n (\nabla \cdot \mathbf{v})$$  \hspace{1cm} (15)$$

where the last term in the right-hand part takes into account the kinematic expansion/compression of matter; the multiplier $(1 - \alpha)$ accounts for the fact that new voids do not arise inside the existing ones. The void growth equation is also modified in order to take into account the simplification of mean void radius discussed above. As well as the radius of new voids $R_c$ differs from $R$, the following correction is necessary for the effective growth rate of the mean radius in comparison with equation (6)

$$\dot{R} = \left(\dot{R}\right)_p - \left(R - \frac{R_c^3}{R^2}\right) \frac{\dot{n}}{n}$$  \hspace{1cm} (16)$$

The formulated equations form the complete system of the tensile fracture of pure metal; all parameters are collected in table 1. Material in an elementary volume is treated as completely fractured if the volume fraction of voids reaches the value $\alpha \geq 0.5$, which is enough for coalescence of adjacent voids and formation of the main crack with high probability. In the completely fractured regions, the pressure is set equal to zero, the density and $\alpha$ are found from the equation of state in order to provide the zero pressure.

### 2.3. Fracture of alloy

It is shown in [30] on the basis of MD simulations that copper inclusions decrease the strength of aluminum matrix due to the stress concentration areas arising near the inclusions at tension; voids grow inside the aluminum matrix near the copper inclusions, but not inside the inclusions. Aluminum alloy D16T (2024) has the second-phase precipitates of nanometer size [33, 34] in its structure, which lead to the same effect [30]. Therefore, generalization of the fracture model described in the previous subsection on the case of alloy can be obtained by taking into account the voids inside the stress concentration areas with higher negative pressure $P_1 = K P$ in comparison with the average pressure $P$, where $K \approx 1.3$ is the stress concentration factor at room temperature [30]. In this case, the total volume fraction of voids is equal to
Table 1. Parameters of fracture model: \( \gamma \) is the surface tension; \( \chi \) is the nucleation work reduction factor; \( \varepsilon_D \) is the energy of dislocation line per unit length; \( \varepsilon_s \) is the formation energy of dislocation from void surface per unit length; \( b \) is the modulus of Burgers vector; \( n_0 \) is the total concentration of the initial voids; \( R_0 \) is the size distribution parameter of the initial voids; \( K \) is the stress concentration factor; \( \alpha_c \) is the volume fraction of the concentration areas; \( Y_0 \) is the static yield strength in material with low dislocation density.

| Parameter          | Al   | D16   | Source |
|--------------------|------|-------|--------|
| \( \gamma \) (J/m\(^2\)) | 2    | 2     | [19]   |
| \( \chi \)         | 0.017| 0.017 | fitted |
| \( \varepsilon_D \) (eV/b) | 5    | 5     | [31]   |
| \( \varepsilon_s \) (eV/b) | 0.136| 0.136 | [19]   |
| \( b \)            | 0.28 | 0.28  |        |
| \( n_0 \) (\(\mu m^{-3}\)) | 0.1  | 100   | fitted |
| \( R_0 \) (nm)     | 0.75 | 1.5   | [30]   |
| \( K \)            | 1    | 1.3   | [30]   |
| \( \alpha_c \)     | 0    | 0.01  | [30]   |
| \( Y_0 \) (MPa)    | 22   | 100   | [32]   |

\[
\alpha = \frac{4\pi}{3} R^3 n + \frac{4\pi}{3} R_1^3 n_1, \tag{17}
\]

where \( R_1 \) and \( n_1 \) are, respectively, the mean radius and concentration of voids inside the stress concentration areas, while \( R \) and \( n \) relate with the main bulk of material outside the inclusions and the stress concentration areas. The volume fraction of stress concentration areas \( \alpha_c \) is about one tenth part of the volume fraction of inclusions, which, in turn, is about several percents. Evolution of \( R \) and \( n \) is described by the set of equations presented in the previous subsection with a sole replacement of the multiplier \( (1 - \alpha) \) by \( (1 - \alpha)(1 - 11\alpha_c) \) in equation (15), which excludes the inclusions and the stress concentration areas. Kinetics of \( R_1 \) and \( n_1 \) is described by the same equations system with replacement of \( P \) by \( P_1 = KP \) and \( (1 - \alpha) \) by \( (1 - \alpha)\alpha_c \).

3. Results and discussion

The formulated system of equations is numerically solved with using of a modification of CRS computer code [35] with accounting of the fracture model described above. Integration of the continuum mechanics equations (1)–(3) is realized by means of the finite-difference numerical method [10]. Other evolution equations are time-integrated by means of simple explicit Euler method. Two problem statements are considered in this paper: (i) tension of a representative volume element with the constant strain rate \( \dot{\varepsilon} \), and (ii) 1D simulation of the high-velocity impact of metal plates. Within the first problem statement, we do not solve the motion equation (2) and set the velocity divergence equal to \( (\nabla \cdot \mathbf{v}) = \dot{\varepsilon} \). This type of calculations is used for obtaining the strain rate dependence of the tensile strength for comparison with MD simulation results [30] and experimentally determined values. The second type of calculations is used for direct comparison with the back surface velocity profiles measured in experiments.

3.1. Strain rate dependences

Figure 1 shows the calculated strain rate dependences of the tensile strength in comparison with MD simulations results [30], the data of the high-velocity impact experiments [36, 37] and the
Figure 1. Strain rate dependences of the tensile strength for pure Al and D16 alloy: comparison of the fracture model results with MD simulations data [30], and data of the high-velocity impact experiments for pure monocrystalline aluminum [36] and annealed D16 alloy [37], as well as experiments [7] on the ultra-short pulse laser irradiation of thin aluminum foils.

Figure 2. Strain rate dependences of the mean void diameter at complete fracture calculated for pure Al and D16 alloy with using the fracture model. This diameter correlates with the size of structural elements on the fracture surface.

experiments [7] on the ultra-short pulse laser irradiation of thin foils (pulse duration is 150 fs). Parameters of the fracture model are determined for both pure aluminum and D16T (2024) aluminum alloy by means of fitting with MD and experimental data; they are presented in table 1. Three parameters, $\chi$, $n_0$ and $R_0$ are varied, while other parameters are taken from previous works [19, 30] or from the reference literature [31, 32]. The nucleation work reduction factor $\chi$ is defined in order to get a correspondence with MD results at ultra-high strain rates ($\geq 10^8$ s$^{-1}$); it has the same value for both pure Al and alloy. In the case of pure Al, the initial voids distribution parameters $R_0$ and $n_0$ are selected from the requirement of correspondence with the impact experiments data [36] for aluminum monocrystals (see figure 1). In the case of alloy, the first parameter, $R_0$, is obtained from the model curve fitting with the data of the impact experiment [37] for D16 alloy, while the second parameter, $n_0$, is chosen in order to obtain the correspondence with the microstructural investigations data [38] for typical sizes of the basic structural elements on the fracture surface. It is shown in [38] that the main level of fracture lies within the range 1 – 5 $\mu$m for D16 alloy at the strain rate above $10^5$ s$^{-1}$, which is in correspondence with the model calculations presented in figure 2 and obtained with using the selected set of parameters shown in table 1. The sizes of structural elements presented in figure 2 are calculated as the mean diameters of voids at the moment of the complete fracture when the voids form the main crack ($\alpha$ becomes greater than 0.5).

Analysis of figure 1 shows that using the proposed fracture model and defined set of parameters one can describe the tensile strength of pure aluminum and alloy within a wide range of strain rates—from $10^5$ s$^{-1}$ to $10^{11}$ s$^{-1}$. At the strain rate less than $10^7$–$10^8$ s$^{-1}$, the main mechanism of fracture is the growth of the pre-existing voids (the growth mode). Concentration of the pre-existing voids become insufficient at the strain rate increase above the mentioned values, and the nucleation of new voids becomes the predominant mechanism.
at the ultra-high strain rates (the nucleation mode). Transition to the nucleation mode leads to reduction of the rate sensitivity of strength and decrease in the slopes of curves in figure 1. The maximal rate sensitivity and curves slopes correspond to the transition region $10^7$–$10^8$ s$^{-1}$ (see figure 1); it correlates with the experimentally observed [39–42] fast increase of the tensile strength at the strain rates above $10^7$ s$^{-1}$ for pure aluminum. Transition to the nucleation mode leads to a drastic decrease of the typical sizes of the fracture surface elements (figure 2) from micrometer-scale down to nanometer-scale.

In the case of alloy, one can see three distinct drops in the strain rate dependences of the fracture element size; two of them correspond to the transition region, while the last one takes place at the strain rates about $10^{11}$ s$^{-1}$. These drops indicate the following changes of the fracture scenario in the course of the strain rate increase: growth of pre-existing voids inside the stress concentration areas around inclusions, growth of pre-existing voids throughout all the volume, nucleation of voids inside the stress concentration areas, and, the last one at highest strain rates, nucleation of voids throughout all the volume.

Figures 3 and 4 show the influence of the size ($R_0$) and concentration ($n_0$) of the pre-existing voids on the strain rate dependences of the tensile strength and the fracture element size, respectively; $K$, $\alpha_c$ and $Y_0$ are taken for pure aluminum.

### 3.2. Back surface velocity profiles

Figure 5 shows the time profiles of the back surface velocity for D16 alloy that are calculated using the proposed fracture model and presented in comparison with the experimental data [37, 43] on the high-velocity impact of metal plates. Calculations are performed in 1D formulation of the problem. In these profiles, one can see the arrival of the elastic precursor at first, the plastic shock front thereafter, the unloading wave, the spall pulse and following reverberations of the spalled layer.
The plasticity model is responsible for the form and height of the elastic precursor and for the unloading wave form [14,22]. The fracture model is responsible for the depth of the spall pulse, first of all. One can see the close positions of the calculated spall pulses to the experimental ones. The advance of the proposed fracture model is that it gives damped reverberations after spallations. These reverberations are much closer in their amplitude and period to that is observed in the experiment in comparison with the previous model [14]. However, a more precise description is necessary for the stage of complete fracture in order to achieve an even better correspondence of the reverberations form. It will be the main direction of further development of the model.

3.3. Comparison with data from short-pulse laser experiments
A number of the tensile strength measurements for aluminum and other materials were performed in [40–42] with using a short-pulse laser irradiation with durations of 2.5 ns and 70 ps and a combined experimental-calculative method with calculation of the shock waves propagation in targets for extracting the tensile strength values. A growth of the strength value together with the intensity of the incident shock wave was reported in [40–42] besides its growth together with the strain rate; this effect was connected by authors with the strengthening due to healing of the initial defects in material under the action of the incident shock wave. As a result, two series of measured points were obtained for two different durations of the laser pulses [42]. It is interesting to compare these results with the developed model; figure 6 presents the corresponding comparison. It seems reasonable that the sharp increase of the strength in both series can be connected with transition from the growth mode to the nucleation mode (see subsection 3.1); this transition can be accelerated by the collapse of the pre-existing pores due to the action of the shock wave. At the same time, the maximal strength values obtained in [40–42] exceed even results of MD simulations for pure monocrystals without pores; this discrepancy looks strange and requires further explanation.
Figure 6. Comparison with data from short-pulse laser experiments: strain rate dependences of the aluminum tensile strength. The plot collects: the fracture model predictions for pure monocrystalline Al and D16 alloy (see figure 1); data of the high-velocity impact experiments for pure monocrystalline aluminum [36] (impact); results of MD simulations of papers [30] (MD), [29] (MD 1), [44] (MD 2) and [45] (MD 3) for pure aluminum; data of experiments [7] on the ultra-short-pulse laser irradiation of thin aluminum foils (laser 150 fs); and data of the short-pulse laser irradiation of aluminum foils for 70 ps (laser 70 ps) and 2.5 ns (laser 2.5 ns) [40–42].

4. Conclusions
A continuum model of tensile fracture is formulated for pure aluminum and D16 alloy basing on the previously obtained results of MD simulations. All equations of the model and the collected and fitted parameters are described in details. The model is used for calculations of the rate dependences of the tensile strength and the typical fracture element sizes within a wide range of strain rates. The results are compared with the existing experimental and MD data.

At the strain rate less than $10^7–10^8$ s$^{-1}$, the main mechanism of fracture is the growth of the pre-existing voids (the growth mode). Concentration of the pre-existing voids become insufficient at the strain rate increase, and the nucleation of new voids becomes the predominant mechanism at the ultra-high strain rates (the nucleation mode). Reduction of the rate sensitivity of strength takes place within the nucleation mode, while the maximal rate sensitivity corresponds to the transition region. Transition to the nucleation mode leads to a drastic decrease of the typical sizes of the fracture surface elements from micrometer-scale down to nanometer-scale.

Comparison of modeling results with the experimental profiles of the back surface velocities for the high-velocity plate impact reveals a satisfactory correspondence in both the spall pulse position and the form of reverberations. More precise description of the complete fracture stage is planned as the main direction of further development of the model.

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