Multi-scale model of the dynamic fracture of molten and solid metals

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Abstract. A multi-scale model of the tensile fracture of metal melts is developed based on a combination of molecular dynamics (MD) simulations and continuum description of kinetics and dynamics of voids; the model considerably extends the time and length scales of MD. Nucleation of voids due to thermal fluctuations is taken into account. Growth of a void in melts is well described by the Rayleigh–Plesset equation, while in the case of a solid metal we propose a dislocation-based model of the void growth. Based on the MD simulations, we investigate the nucleation rates in the uniform monocrystalline metals and metal melts, dynamics of pre-existing voids and compare them with the continuum model (equations of nucleation and growth). Using of the literature data on the surface tension and viscosity of melts allows us to get a correspondence between the continuum description and MD. With the use of the model, we calculated the strength of the uniform melts of Al, Cu, Ni, Pb, Fe and Ti within a wide range of strain rates (from $10^3$–$10^4$ to $10^9$–$10^{11}$ s$^{-1}$) and temperatures (from melting temperature to 70–80% of critical temperature). Calculations show that the tensile strength of homogeneous melts decreases slowly with the strain rate decrease. As a result, within the range of strain rates of $10^6$–$10^8$ s$^{-1}$, a homogeneous nucleation mode can be realized, in which the dynamic strength of a melt can be comparable to, or even higher than the strength of a solid metal.

1. Introduction
Dynamic tensile fracture is most often considered in solid metals [1–4], while it can also take place in metal melts [5–7]. Solid metals and metal melts 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) from a free surface or release of heated matter in the energy absorption zone of a powerful laser [5,7–9] or a high-current electron beam [10–13]. Decay of this metastable state is the tensile fracture, which is realized by means of nucleation and growth of voids.

Development of a fracture model applicable in a wide range of strain rates and thermodynamic parameters is a topic of high importance for interpretation of the existing experimental data and using in the mathematical modeling of dynamic processes [14–16]. Fracture models used in continuum simulations are based on various model equations for growth of some damage parameters. The equations can have a more or less complex form, but they all require parameters obtained traditionally from the experimental data. Another powerful tool in theoretical investigations of fracture is molecular dynamics (MD) [17–21], which is as much precise as accurate the used interatomic potentials are. A substantial restriction for MD is the accessible scale of lengths and times, which allows investigating directly only very high strain rates—typically above $10^8$ s$^{-1}$. Integrating model equations for damage (voids) with MD simulations

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is a promising direction in theoretical investigations of fracture [19, 20].

In the present paper, we report our progress in the development of a multi-scale model of fracture of metals and metal melts at high-rate tensile deformation. The model describes the dynamic deformation of materials at the macro-level using the continuum mechanics framework; meanwhile, the evolution of ensembles of voids is described at the micro-level using the equations of nucleation, growth and interaction of voids; these equations supplement the macroscopic equations. The equations of void evolution and their parameters are obtained from the results of molecular dynamics simulation.

2. Continuum mechanics

Here we describe how the ensemble of cavities is taken into account within the continuum mechanics equations. We neglect the vapor, which can occur inside cavities at high temperatures of the melt; in this approximation, we have a single condensed phase with empty cavities (voids). According to [15, 21], the presence of defects can be taken into account by means of an additional tensor $W_{ik}$ of the material deformation at the expense of formation and growth of defects. In this case, the basic continuum mechanics equations have the following form:

$$\frac{1}{\rho} \frac{d \rho}{dt} = - \sum_{k=1}^{N} \left( \frac{\partial v_k}{\partial x_k} + \frac{dW_{kk}}{dt} \right),$$  \hspace{1cm} (1)$$

$$\rho \frac{d v_i}{dt} = \sum_{k=1}^{N} \frac{\partial}{\partial x_k} (- P \delta_{ik} + S_{ik}),$$  \hspace{1cm} (2)$$

$$\rho \frac{d U}{dt} = \sum_{k=1}^{N} \left[ -P \left( \frac{\partial v_k}{\partial x_k} + \frac{dW_{kk}}{dt} \right) + \sum_{i=1}^{N} S_{ik} \frac{d w_{ik}}{dt} \right],$$  \hspace{1cm} (3)$$

where $\rho$ is the true density of the substance (with the exception of voids), $x_k$ are the Cartesian coordinates, $v_i$ are the components of the substance velocity, $P$ is the pressure, $S_{ik}$ are the stress deviators, $U$ is the internal energy, $w_{ik}$ is the tensor of plastic deformation [15, 22], subscripts $i$ and $k$ denote the spatial directions, $N$ is the dimension of the problem, $\delta_{ik}$ is the bivalent mixed tensor. The Lagrange frame of reference is used in equations (1)–(3). In the case of solid metal, the stress deviators $S_{ik}$ and the plastic deformation $w_{ik}$ is calculated using the dislocation plasticity model [15, 22]; in the case of melt, they are zero: $S_{ik} = 0$ and $w_{ik} = 0$.

The fracture model should construct the tensor of fracture deformation $W_{ik}$. Supposing that voids have a spherical shape and can be divided in generations [23] with similar radii in each generation due to the close time of evolution, one can write the following equation for this tensor [21]:

$$\frac{d W_{ik}}{dt} = - \delta_{ik} \frac{1}{3} \frac{1}{1 - \alpha} \frac{d \alpha}{dt},$$  \hspace{1cm} (4)$$

where $\alpha$ is the volume fraction of voids:

$$\alpha = \sum_{m=1}^{M} \left( \frac{4\pi}{3} R_{m}^{3} n_{m} \right),$$  \hspace{1cm} (5)$$

where the subscript $m$ numerates all generations, $M$ is the current number of generations, $R_{m}$ is the void radius of the generation with number $m$, $n_{m}$ is the corresponding concentration (the number of voids per unit volume of the substance). Equations for $R_{m}$ and $n_{m}$ are necessary for closing the model.
3. Tensile fracture of melt

3.1. Model for melt

In the case of a melt at negative pressure, we have a classical problem of cavitation in a metastable liquid [24]. The change in the radius of existing cavities is described by the Rayleigh–Plesset equation [20]:

\[
d\frac{2R_m}{dt^2} = \frac{3}{2} \frac{1}{R_m} \left( \frac{dR_m}{dt} \right)^2 + \frac{1}{R_m \rho} \left[ -P - \frac{2\sigma}{R_m} \right] - \frac{4\eta}{\rho} \frac{1}{R_m} \left( \frac{dR_m}{dt} \right),
\]

where \(\sigma\) is the surface tension, \(\eta\) is the melt viscosity. As it follows from equation (6), a cavity can grow if it has a radius larger than the critical value \(R_c = 2\sigma/(-P)\) (the pressure should be negative). Formation of such a cavity demands the following work against the surface tension:

\[
W_c = \frac{(16\pi/3)\sigma^3}{P^2}.
\]

The probability of corresponding thermal fluctuation [25] is equal to \(\exp(-W_c/(k_BT))\), where \(k_B\) is the Boltzmann constant, \(T\) is the melt temperature. Therefore, the rate of concentration variation due to the homogeneous nucleation of voids can be written as follows:

\[
\frac{dn_{m}}{dt} = \delta_{mM} f \alpha^{-3} \exp \left( \frac{-16\pi \sigma^3}{3k_BT P^2} \right) (1 - \alpha),
\]

where \(\alpha\) is an average interatomic distance, which is calculated from the density; \(f = 100 \times c/a \approx 10^{14}\) Hz, \(c\) is the sound velocity in the melt. The bivalent mixed tensor \(\delta_{mM}\) means that the homogeneous nucleation leads to the formation of cavities of only the youngest generation, the number of which is \(M\). In calculations, if the critical radius change is more than 0.05%, then a new generation is introduced.

3.2. Parameters of model

Surface tension is the main parameter determining the tensile strength of the melt. For little voids with size comparable with \(a\), the dependence of surface tension on radius should be taken into account, which can be approximated by Tolman’s formula [20]:

\[
\sigma = \frac{\sigma'}{1 + a/(2R_m)},
\]

where \(\sigma'\) is the surface tension for a flat surface. In accordance with [26], the surface tension of the melt decreases linearly with temperature:

\[
\sigma' = \sigma_m - K_{\sigma} (T - T_m),
\]

where \(\sigma_m\) is the surface tension at the melting temperature \(T_m\); the coefficient \(K_{\sigma}\) is the absolute value of the derivative of surface tension over temperature, which is assumed to be a constant. As the surface tension should be zero at the critical temperature \(T_K\), this constant can be found as \(K_{\sigma} = \sigma_m/(T_K - T_m)\). According to [27], the following approximation can be used for the dependence of viscosity of liquid metals on density:

\[
\eta = \frac{\eta_0}{\rho_\infty / \rho_t - 1},
\]

where \(\eta_0\) is a parameter with the dimensionality of viscosity, \(\rho_\infty\) is the substance density, which corresponds to the infinitely high viscosity and zero fluidity [27]. Table 1 summarizes the parameters for Al, Cu, Ni, Pb, Fe and Ti. Metastable forms of the wide-range equations of state [28–31] are used to determine thermodynamic properties of matter.
Table 1. Parameters for calculating the surface tension and viscosity, and references to equations of state [26–30, 32].

| Parameter | Cu       | Al       | Ni       | Pb       | Fe       | Ti       |
|-----------|----------|----------|----------|----------|----------|----------|
| $\sigma_m$ (J/m$^2$) [26] | 1.031    | 1.352    | 1.810    | 0.460    | 1.180    | 1.520    |
| $K_\sigma$ (mJ/(m$^2$K)) | 0.146    | 0.192    | 0.242    | 0.105    | 0.260    | 0.260    |
| $T_m$ (K) [26] | 933      | 1358     | 1728     | 601      | 1830     | 1933     |
| $T_K$ (K) [28, 32] | 8000     | 8390     | 9460     | 4980     | 6500     | 7600     |
| $\eta_0$ (µPa s) [27] | 91       | 435      | 645      | 114      | 490      | 100      |
| $\rho_\infty$ (g/cm$^3$) [27] | 2.70     | 8.95     | 8.76     | 11.32    | 7.45     | —        |
| Equation of state | [28] | [28] | [29, 30] | [28] | [28] | [29, 30] |

3.3. Tensile strength of melts

For calculation of tensile strength, we consider a model problem of melt tension at constant temperature (in thermostat) and at a constant strain rate $\dot{\varepsilon}$. It means, that in the framework of the discussed model, equations (1) and (3) are not solved, and the velocity divergence $\sum_{k=1}^{N}(\partial v_k/\partial x_k)$ in equation (2) is replaced by $\dot{\varepsilon}$. Additional calculations have shown that strength is determined by the melt temperature at the instant of fracture and does not depend on the previous history of temperature variations. Therefore, the isothermal approximation does not distort the data.

Results of the described model are compared with the results of MD simulations. In the last case, we use the parallel molecular dynamics simulator LAMMPS [33] with the interatomic potentials: [34]—for Al and Cu; [35]—for Ni, Pb, Fe and Ti. The uniform uniaxial tension was modeled by the scaling of coordinates of atoms [33]; the system was in a thermostat at constant temperature; periodic boundary conditions were set for all boundaries. Most of the calculations were performed with the systems of 108,000 atoms (for the strain rates of $10^9$ s$^{-1}$ and $10^{10}$ s$^{-1}$) and 500,000 atoms (for the strain rate of $10^8$ s$^{-1}$). Additional calculations with larger and smaller systems show that these numbers of atoms are large enough to obtain the value of tensile strength with a precision of about several percent.

At the initial stage of deformation, the melt is homogeneous; a negative pressure therein increases monotonically in modulus. At a sufficiently high level of tensile stresses, formation of cavities and their growth begin. Over time, the growth rate of the volume of the cavities in the melt starts to exceed the rate of increase of the system volume, the decrease in the melt density changes to its increase, and the pressure, on the contrary, reaches a maximum and begins to decrease (in the absolute value). The maximum value of the negative pressure modulus is the melt strength. Similar behavior is observed both in the case of continuum model and in the case of MD simulations.

A clear correspondence between the MD and the continuum model is observed in the strength behavior with variation of temperature or strain rate. This correspondence obtained for six metals (Al, Cu, Ni, Pb, Fe, Ti) evidences the adequate description within the framework of the continuum model. Moreover, there is a quantitative correspondence, which can be interpreted as mutual verification of the literature data used for the model parameters (table 1) and the used interatomic potentials [34, 35]. An example of comparison between the MD data and the results of the continuum model is shown in figure 1 for the case of iron.

A comparison with experimental data for strength of Al and Ni melts is also made. Experimental data are very rare in this field, but recent experiments on the ultra-short laser
irradiation of metal foils gave some information [5,6]. For the case of Al, the experimental value (2.5 ± 0.5 GPa at 2500 K and 10^{10} \text{s}^{-1} [6]) coincides with the calculation results. For the case of Ni, the experimental value (6 ± 1 GPa at 3500 K and 10^{9} \text{s}^{-1} [6]) is on 2 GPa higher than the calculated one.

With the use of the continuum model, we calculate the strength of the uniform melts of Al, Cu, Ni, Pb, Fe and Ti within a wide range of strain rates (from 10^{3} – 10^{4} to 10^{9} – 10^{11} \text{s}^{-1}) and temperatures (from melting temperature to 70–80% of critical temperature). An example of calculations in the case of Fe is shown in figure 2. Calculations show that tensile strength of the homogeneous melt decreases slowly with decrease in the strain rate.

### 3.4. Rate of nucleation and dynamics of voids

Here we compare the nucleation rates calculated using the continuum model (equation (7)) and the results of MD simulations. For convenience, the nucleation rate is expressed as the number of events per atom per 1 ps in both cases. In the MD simulations, an initially uniform system is constrained at the constant volume and temperature; the volume is excess in order to provide an expanded state of matter with negative pressure. We determine the life time $\tau$ of the melt existence in this state till the formation of cavities, which brings the system out of the metastable state. Several MD trajectories are calculated for each set of temperature and initial pressure, and an average life time $\langle \tau \rangle$ is calculated. Then, the strain rate is a reciprocal to the average life time: $Y_{MD} = 1/ (\langle \tau \rangle N_a)$, where $N_a$ is the number of atoms in the MD system.

Figure 3 shows the results of comparison for the nucleation rate. As the nucleation rate exponentially depends on pressure and temperature, even small variations in the thermodynamic parameters result in a sharp change of the nucleation rate by orders of magnitude. As one can see, there is a certain correspondence between MD and the continuum model, especially in the range of 1500–2000 K, but the correspondence is not so good as for the values of strength (see figure 1). The continuum model underestimates the strain rate in comparison with MD at lower temperatures and overestimates it at higher temperatures. However, this misfit does not prevent correct determination of tensile strength in the framework of the continuum model (see figure 1). It is explained by a weak influence of the nucleation rate on the value of strength. An additional investigation using the continuum model shows that changing the nucleation rate by

**Figure 1.** Tensile strength of iron melt versus temperature at strain rates of 10^{9}, 10^{10} \text{s}^{-1}: molecular dynamics (markers) and continuum model (lines).

**Figure 2.** Tensile strength of iron melt versus strain rate and temperature; calculations are on the basis of the continuum model.
two orders of magnitude results in the change of tensile strength in the range of 10%. The reason is the following: regardless of the nucleation rate, the cavities form as long as there are conditions necessary for nucleation. This process results in the formation of a certain concentration of voids, and it is not so important, how much time precisely is necessary for the process of nucleation.

We also compare the results of the continuum modelling and the MD simulations for the evolution of volume of a pre-existing void in the melt expanded at a constant strain rate. Figure 4 presents the results for the aluminum melt at temperature 1000 K and strain rate of $10^9$ s$^{-1}$. Using of periodic boundary conditions in MD means that we have a system of pores (with concentration of $7 \times 10^4\,\mu\text{m}^{-3}$) rather than a single pore; therefore, the change in the volume of voids influences the pressure in the system. The same formulation is used in the continuum model.

At zero pressure in the system, the void is unstable and its volume begins to reduce (figure 4a) under the action of surface tension. Negative pressure changes the reduction into growth of void. Then, some oscillations of the cavity take place against the background of gradual increase in its volume connected with the expansion of the system. The pressure oscillates around zero level (figure 4b). The results of MD and the continuum model agree with each other up to the time of 12 ps, when the volume fraction of voids reaches 6% and the void diameter reaches the value of a quarter of distance between centers of voids. A subsequent discrepancy can be explained by a mutual influence of adjacent pores, which is not taken into account in the continuum model. At the same time, the character of the behavior coincides for MD and the continuum model. The initial segment of the curve up to the beginning of the pressure growth (designated by the level “fracture” in figure 4) is the most important for the fracture model; there is a good correspondence between MD and the continuum model at this initial stage.

4. Fracture of solid metals
The behavior of solid metals is more complex than the behavior of liquids. Growth of elementary deformation centers (pores) is controlled by the processes of plastic deformation, in particular, the kinetics of formation of dislocations near cavities. Using the molecular dynamics simulator LAMMPS [33], we study the growth of pre-existing pores and nucleation of pores in the initially uniform solid metal. It allows us to formulate the models of growth and nucleation described in the following subsections.
4.1. Growth of voids in solids

MD simulations demonstrate that nanovoids in solid grow through plastic deformation around the void. We assume that the volume change of the void is entirely defined by plastic deformations in the zone, where shear stress exceeds the static yield strength of the material \( \sigma_\tau \geq Y/2 \). The radius of this zone can be estimated by solving the equilibrium equation in the case of spherical symmetry [36]:

\[
    r_{pl} = R_m \left( \frac{2\sigma_{\tau}^{\text{max}}}{Y} \right)^{1/3},
\]

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

\[
    \frac{dR_m}{dt} = \frac{dw}{dt} (r_{pl} - R_m).
\]

Plastic strain rate \( w \) can be found from the Orowan equation [37]:

\[
    \frac{dw}{dt} = \frac{b}{\sqrt{6}} V_D \rho_D,
\]

where \( b \) is the Burgers vector magnitude, \( V_D \) is the dislocation velocity, \( \rho_D \) is the scalar density of dislocations. A stationary form of the equation of dislocation motion can be used:

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

where \( B \) is the phonon friction coefficient, \( c_t \) is the transverse sound velocity.

As follows from the MD results, the nucleation of dislocations near the 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 [38] and introduce the following equation of the dislocation density balance:

\[
\frac{d\rho_D}{dt} = 2\pi c_l n_m \exp \left( -\frac{U - V_0\sigma_{\text{max}}}{k_B T} \right) + \frac{0.1}{\varepsilon_D} (b\sigma_{\text{max}} V_D) \rho_D,
\]

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 the voids in the substance \(n_m\)) by the length of the dislocation segment \(2\pi R_m\) arising in one nucleation act and by the characteristic frequency, which can be estimated as \(c_l/R_m\). 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 [15, 22], \(\varepsilon_D = 8\text{ eV}/b\) is the dislocation formation energy per unit length.

4.2. Nucleation of voids in solids
The model of growth gives us the following value of the critical void radius: \(R_c = 2\sigma/(|P| - 2Y/3)\); a larger void can grow due to the motion of existing dislocations or nucleation of new dislocations. As usually \(|P| \gg 2Y/3\), a simpler expression can be used instead: \(R_c = 2\sigma/(-P)\), which is similar to that in the case of the melt. The work of a void formation can be estimated as [21]: \(W_c = (16\pi/3)\sigma^3/P^2\), which also coincides with the case of the liquid. Thus, the nucleation rate can be calculated by equation (7).

Figure 5 shows the comparison of the nucleation rates calculated by equation (7) and from the MD simulations for solid monocrystalline aluminum at several temperatures. The problem statement is the same as in subsection 3.4. In the case of the solid, one can see even better correspondence between the continuum model and MD than in the case of the melt (compare with figure 3).

5. Conclusions
A multi-scale model of tensile fracture of solid metals and metal melts is developed based on a combination of molecular dynamics (MD) simulations and continuum description of kinetics and
dynamics of voids. The model develops the classical nucleation-and-growth (NAG) approach [39] and considerably extends the time and length scales of MD. Nucleation of voids is described in the framework of the theory of thermal fluctuations uniformly for solid metals and metal melts. Growth of a void in a melt complies with the Rayleigh–Plesset equation, while in the case of a solid metal we propose a dislocation-based void growth model. In contrast with the model that was proposed in [20] for a Lennard-Jones liquid, our model takes into account the feedback of voids growth on the stressed state and considers a number of metal melts with a more complex interactions between atoms. As opposed to MD investigations that was presented in [19] for solid aluminum, here we propose explicit equations describing the plasticity-driven growth of voids on the basis of dislocation approach. These equations also allow one to take into account initial dislocation density, it means, the initial state of metal. Values of tensile strength of Al and Ni melts that are calculated with the use of the multi-scale model are compared with the experimental data from [5, 6]. For the case of solid metals, the comparison of the calculated strength values with the experimental data from literature for a wide range of strain rates will be the next stage.

Using of the model, we calculated the strength of homogeneous melts of aluminum, copper, nickel, lead, iron and titanium in a wide range of strain rates (from 1–10/ns to 1–100/ns) and temperatures (from melting temperature to 70–80% of critical temperature). Calculations show that the tensile strength of the homogeneous melt decreases slowly with decrease in the strain rate. As a result, in the range of strain rates of 0.001–0.1/ns, a homogeneous nucleation mode can be realized, in which the dynamic strength of the melt can be comparable or even higher than the strength of the solid metal at room temperature.

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