# Dynamic fracture of metals in wide range of strain rates

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**Abstract** A model of dynamic tensile fracture is constructed, which is applicable for many metals in wide range of strain rate. It considers a stage of thermofluctuation nucleation of voids and stages of voids growth and aggregation. The model contains two fitted parameter for each substance: the first parameter is a specific free energy of metal surface; the second one is a distribution parameter for weakened zones of material. These parameters are found for copper, aluminum, iron, titanium, nickel and molybdenum by fitting with the experimental data and molecular-dynamics simulations. Calculations show that there are two regions with different slope in the strain rate dependence of strength: in the first one (at strain rate $< 10^8$ $s^{-1}$) voids are nucleated in weakened zones, and strength grows up relatively fast with strain rate; in the second one (at strain rate $> 10^8$ $s^{-1}$) number of weakened zones becomes insufficient, voids are nucleated predominantly in perfect material, and the strength growth is decelerated. Plasticity is not effect on voids nucleation and on the material strength at the strain rate $> 10^7$ $s^{-1}$, but it becomes a dominant factor at the strain rate $< 10^4$ $s^{-1}$.

**Keywords** Fracture, High-rate tension, Metal, Micro-cracks, Two-level approach

## 1. Introduction

Dynamical tensile strength is an important property of materials. A number of experimental works is devoted to its determination: a plate impact [1,2], a short-pulse laser irradiation [3-5] and a powerful ion irradiation [1] can be used to produce conditions of metal rupture. Very high strain rates (above $10^9$ $s^{-1}$) are available now in experiments on irradiation of thin foils by short laser pulses [3,5]. Molecular dynamics (MD) is also a useful method for the investigation of fracture at ultra-high strain rates [6-10]. The dynamical strength value substantially depends on the strain rate. Experiments and MD simulations can not cover all possible ranges of this parameter. Therefore, their data have to be supplemented by some approximation for using in simulations of dynamical processes in materials. For example, the strain rate dependence of the dynamic strength is commonly approximated by a simple power law [3,10]).

Various physical models of fracture typically separate the stages of the voids nucleation and of the voids growth [11]. Nucleation of voids is strongly effected by the presence of inclusions, grain boundaries and other defects of the crystal structure [12].

A modification of the model [13] is presented here, which considers weakened zones of material with reduced threshold of the micro-voids generation. It allows describing the strain rate dependence of strength in the range of strain rates from $10^3$ $s^{-1}$ up to $10^{11}$ $s^{-1}$. Kinetics of the dynamic fracture of metals is numerically investigated basing on the proposed model.

## 2. Model of fracture

The model uses two-level approach for fracture description. Micro-level of modeling deals with individual micro-cracks in crystalline material and describes their thermo-fluctuation nucleation, growth and aggregation. Macro-level deals with averaged values through a length scale much large the distance between the cracks. Micro-cracks growth is described with use of simplified dynamics

equation for its radius. Macro-level is described by continuum mechanics equations with additional terms, which takes the micro-cracks ensemble into account.

### 2.1. Voids growth equation

Let $\vec{\beta}$ to be a unit vector directed along the maximal tensile stress. Tensile stress $\sigma_\beta = \sigma_{ik}\beta_i\beta_k$ can initiate formation and growth of the opening mode cracks perpendicular to $\vec{\beta}$ (see Fig. 1). Let us consider such a micro-crack, which is supposed to be isolated and axially-symmetrical. Radius of crack is $R$ and its half-thickness is $h$; its volume $V_\mathrm{f}$ can be estimated as a volume of cylinder $V_\mathrm{f} = \pi R^2 \cdot 2h$. Opening of crack creates non-uniform field of displacements in its vicinity. Created by a localized disturbance, the displacements have to decay with distance with on the scale $R$. Maximal displacements in $\vec{\beta}$ direction corresponds to the crack faces, and it is $+h$ and $-h$ for opposite faces. Therefore, the ratio $h/R$ can be used as an estimation of the strain value in the crack vicinity. Corresponding stress can be estimated as $G(h/R)$. In the loaded medium this internal stress is superposed on the external macroscopic tensile stress $\sigma_\beta$. And the total stress has zero normal components on the crack faces to maintain the constant form at the fixed radius $R$. Hence, we obtain an estimation $h = R\sigma_\beta / G$ for the crack half-thickness; than the crack volume is $V_\mathrm{f} = 2\pi R^3 \sigma_\beta / G$. Usage of the last two formulas assumes that the crack thickness instantly adapts to variations of $R$ or $\sigma_\beta$ (a quasi-static approximation), it is valid when the typical time of variations $\tau$ ($\tau \approx R/\dot{R}$ or $\tau \approx 1/\dot{\varepsilon}$, where $\dot{\varepsilon}$ is the strain rate) is much longer than the transient period $R/c_t$. Therefore, conditions for the quasi-static approximation are the next: $\dot{R} \ll c_t$ and $\dot{\varepsilon} \ll c_t / R$; these inequalities usually take place.

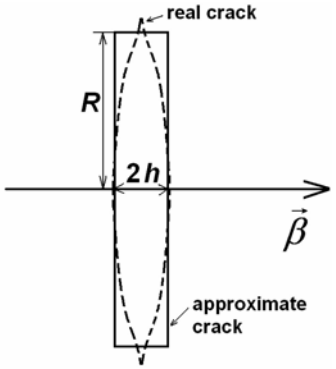


Figure 1. A separate micro-crack; the real crack shape is approximated by cylinder.

The crack grows due to separation of atoms along the plane of crack. The growth rate is restricted by inertia of the surrounding material. It is possible to formulate a Lagrange equation [14] for the micro-crack growth, using the radius $R$ as a generalized coordinate. In this approach system is characterized by the Lagrange function $L = K - U_S - U_V$, where $K$ is the kinetic energy of the substance movement due to the growth of micro-crack; $U_S$ is the surface energy of the crack faces; $U_V$ is the potential energy of crack in the field of external stresses $\sigma_\beta$, and by the dissipative function $F$, which is equal to the one half of the mechanical energy decrease rate due to plastic deformation in the micro-crack vicinity. Expression $K = \rho V_\mathrm{f} \dot{R}^2$ is used as an estimation of the

kinetic energy, where $\rho$ is the density of substance. Work of the external stresses $\sigma_\beta$ at the crack opening is equal to the work on the crack faces; its work on the bulk is zero because of symmetry. One can integrate the elementary work along faces and obtain the value $\sigma_\beta \cdot \delta V_{\mathrm{f}}$, where $\delta V_{\mathrm{f}}$ is an increment of the crack volume. Therefore, the potential energy of crack in the external stress field $\sigma_\beta$ can be written as $U_V = -\sigma_\beta V_{\mathrm{f}} = -2\pi R^3 \sigma_\beta^2 / G$; negative sign here indicates that the micro-crack growth is energy-wise efficient in the tensile stress. Potential surface energy connected with two crack faces is equal to $U_S = 2\pi R^2 \gamma$.

Estimation of the dissipative function is more complex. The crack size changing is accompanied by generation of non-uniform fields of deformations and stresses in the crack vicinity, and the shear part of these stresses undergoes plastic relaxation. Due to the plastic strain the mechanical energy of the growing or collapsing crack is conversed in heat. On the base of the Orowan equation for dislocation plasticity, one can write the maximal plastic strain rate $\dot{w} = b \rho_D c_t$, where $\rho_D$ is the scalar density of dislocations in the substance, $b$ is the modulus of the Burgers vector of dislocations, $c_t$ is the limiting speed of the dislocations movement. Using the ratio $h/R = \sigma_\beta / G$ as a characteristic value of deformation in the crack vicinity, we obtain a characteristic time of the plastic relaxation $\tau_D = (h/R)/\dot{w} = \sigma_\beta / (G b \rho_D c_t)$. This is a time interval sufficiently large for the plastic relaxation of excess shear stress in the crack vicinity if the form of crack is artificially frozen. Then the mechanical energy decrease rate can be estimated as $K/\tau_D$ (external stresses and, respectively, $U_V$ are supposed to be fixed). Than the dissipative function is equal to $F = (1/2) K / \tau_D = \pi\rho (b\rho_D c_t) R^3 \left(\dot{R}\right)^2$.

Substituting all obtained elements in the Lagrange equation, one can obtain the next equation for the crack radius:

$$\rho \frac{\sigma_\beta}{G}\left( R^2 \ddot{R} + \frac{3}{2} R \left(\dot{R}\right)^2 \right) = -4(\gamma + \gamma') + 6R \frac{\sigma_\beta^2}{G}, \qquad (1)$$

where $\gamma' = (\rho/2)(b\rho_D c_t) R^2 \dot{R}$ is irreversible energy (per unit area of crack faces) spending on plastic deformations; this energy dissipates both at the growth and at the collapse of the crack. It follows from the Eq. (1), that the crack grows when its radius exceeds a critical value $R_{\mathrm{cr}} = (2/3) G \sigma_\beta^{-2} (\gamma + \gamma')$. Calculations show, that at high-rate deformation the value of $\gamma'$ is negligible with respect to $\gamma$ for just formed cracks with critical radius. Therefore, initial crack growth occurs in a brittle mode, practically without energy dissipation on the plastic deformations. In particular, the next relation is valid with good accuracy $R_{\mathrm{cr}} = (2/3) \gamma G \sigma_\beta^{-2}$. But at the micro-crack growth, the irreversible energy $\gamma'$ increases and it can reach the value of the order of : $1000\ \mathrm{J/cm^2}$ for large cracks, which exceeds the value of $\gamma$ on the three orders of magnitude.

### 2.2. Nucleation of cracks. Weakened zones of the material

Let us consider a micro-cracks ensemble. We denote the number of micro-cracks in unit volume of substance as $n$. To find the micro-cracks production rate we assume, that all they are generated due to thermal fluctuations. We assume that main contribution in $dn/dt$ is provided by cracks with critical radius $R_{\mathrm{cr}}$, because cracks with $R < R_{\mathrm{cr}}$ are being healed, and generation of cracks with

$R > R_{\text{cr}}$ is the low-probability process. Formation work for critical crack is $A_{\text{cr}} = U_V\left(R_{\text{cr}}\right) + U_S\left(R_{\text{cr}}\right)$ (it is reversible process without plastic dissipation), and we obtain $A_{\text{cr}} = \left(2/3\right)\pi \cdot \gamma \cdot R_{\text{cr}}^2$. The probability of such fluctuations is $P = \exp\left(-A_{\text{cr}} / \left(k_B T\right)\right)$ [16], where $T$ is the substance temperature, $k_B$ is the Boltzmann constant.

Concentration of the fluctuating centers can be estimated as $n_{\text{g}} = 1/\left(8R_{\text{cr}}^3\right)$. Fluctuation frequency $f$ can be estimated as the frequency of transverse phonon with wavelength equal to the critical crack diameter $f = c_t / \left(2R_{\text{cr}}\right)$. As a result, the cracks nucleation rate is

$$\frac{dn}{dt} = P \cdot n_{\text{g}} \cdot f = \frac{c_t}{16R_{\text{cr}}^4} \exp\left(-\frac{2\pi \cdot \gamma \cdot R_{\text{cr}}^2}{3k_B T}\right). \tag{2}$$

The Eq. (2) determines the nucleation rate in the pure, defect-free material. In the real solids there are structural defects, such as dislocations, grain boundaries in polycrystals, inclusions in alloys etc. Micro-crack formation in the defective (weakened) regions requires smaller work in comparison with the undefective one, since these regions already possess raised energy relative to the defect-free crystal material (atoms in it are weaker bounded with each other). Primary origination of voids near the defects is observed in MD simulations [7,10]. We have to consider an influence of defects on the micro-cracks formation. Faultiness of current region of the material can be characterized by a parameter $\gamma^*$ in such a way, that difference $\left(\gamma - \gamma^*\right)$ defines the crack surface formation energy per unit area in this defective region, $\gamma^* < \gamma$. Then the formation work of the critical crack is equal to $A_{\text{cr}}\left(\gamma^*\right) = \left(2/3\right)\pi\left(\gamma - \gamma^*\right)R_{\text{cr}}^2$, where $R_{\text{cr}}$ is determined by $\gamma$ because the crack must grow further in the defect-free regions of crystal, hence, it should be stable at this value of surface tension. We suppose that the weakened zones are exponentially distributed on $\gamma^*$: $n\left(\gamma^*\right) = n_0 \cdot \exp\left(-\gamma^* / \Delta\gamma\right)$ where $\Delta\gamma$ is a distribution parameter. The product $n\left(\gamma^*\right)d\gamma^*$ is the number of micro-cracks nucleation centers in unit volume of substance with the faultiness parameter belonging to $d\gamma^*$ interval near the $\gamma^*$. The constant $n_0$ is determined by the normalization condition: $n_g = \int_0^{\gamma} n\left(\gamma^*\right)d\gamma^* = n_0 \cdot \Delta\gamma \cdot \left(1 - \exp\left(-\gamma / \Delta\gamma\right)\right)$. Than the crack generation rate is defined by the following expression:

$$\frac{dn}{dt} = \frac{c_t}{16R_{\text{cr}}^4} \frac{\left[\exp\left(-\left(2\pi\,\gamma\,R_{\text{cr}}^2\right)/\left(3k_B T\right)\right) - \exp\left(-\gamma/\Delta\gamma\right)\right]}{\left[1 - \left(2\pi\,\Delta\gamma\,R_{\text{cr}}^2\right)/\left(3k_B T\right)\right] \cdot \left[1 - \exp\left(-\gamma/\Delta\gamma\right)\right]}. \tag{3}$$

At $\Delta\gamma = 0$ (homogeneous material) this equation turns back to the Eq. (2). Thus, the proposed model of fracture contains two empirical parameters: $\gamma$ and $\Delta\gamma$. The first of them, $\gamma$, is of the order of surface tension, and the second one, $\Delta\gamma$, is defined by the degree of material faultiness.

### 2.3. Continuous formulation

Here and further we operate with macroscopic length scale, which is much larger than the micro-crack size and the distance between the micro-cracks. It means that each physically small volume of substance contains a set of micro-cracks. Therefore, we use macroscopic fields of substance density, velocity, stresses, deformations, et alia, which are averaged over such physically small volumes. Let us assume that in considered substance element all micro-cracks have identical

spatial orientation $\vec{\beta}$. For volume element $V$ it is possible to write: $V = V_c + V_{Sf}$, where $V_c$ is a part of volume occupied by solid, not cracked, material, and $V_{Sf}$ is a total volume of all micro-cracks in $V$. Let us introduce $\eta = V_{Sf}/V$ – the fraction of volume which is occupied by cracks. Growth of the total micro-cracks volume with rate $\dot{V}_{Sf}$ at the fixed total element volume $V$ leads to decrease of the solid material volume with the rate $\dot{V}_c = -\dot{V}_{Sf} = -V \cdot \dot{\eta}$. If $h << R$, than this change of solid material volume occurs predominantly due to solid material deformation in the $\vec{\beta}$ direction. Corresponding deformation of substance in auxiliary coordinate system is characterized by a sole strain component:

$$\frac{dW_{\beta\beta}}{dt} = \left.\frac{\dot{V}_c}{V_c}\right|_{V=const} = -\frac{1}{1-\eta}\frac{d\eta}{dt},$$

Transformation of this strain tensor into lab coordinates is the next:

$$\frac{dW_{ik}}{dt} = -\beta_i\beta_k\left(\frac{1}{1-\eta}\frac{d\eta}{dt}\right), \tag{4}$$

where $W_{ik}$ is symmetrical strain tensor. The use of $W_{ik}$ as an additional strain of solid material allows considering of the tensile stresses relaxation caused by cracks nucleation and growth. Assuming that all micro-cracks in volume element have the same size, it is possible to write for the micro-cracks volume fraction $\eta = n \cdot V_f$.

The adjacent micro-cracks can coalesce forming a main crack or fractionized zone of material. We suppose that separate micro-cracks develop solitary until their diameter $2R$ reaches the value of an average distance between the cracks, which is equal to $n^{-1/3}$. If the relation $2R \geq n^{-1/3}$ is satisfied in any volume element, then material of this element is assumed to be completely fractured, and all stress components are set equal to zero in it.

In the present report a uniaxial deformation of substance along *Oz*-axis is considered with the constant macroscopic strain rate $d\varepsilon_{zz}/dt = \text{const}$. The maximal tensile stress operates along *Oz*-axis: $\vec{\beta} = \vec{e}_z$, $\sigma_\beta = \sigma_{zz}$. The continuum mechanics equations in this case are reduced to the next set:

$$\frac{d\rho}{dt} = -\rho\left(\frac{d\varepsilon_{zz}}{dt} + \frac{dW_{zz}}{dt}\right), \tag{5}$$

$$\rho\frac{dU}{dt} = \sigma_{zz}\left(\frac{d\varepsilon_{zz}}{dt} + \frac{dW_{zz}}{dt}\right) + S_{zz}\frac{dw_{zz}}{dt}, \tag{6}$$

$$\sigma_{zz} = -P(\rho, U) + S_{zz}, \tag{7}$$

$$\frac{dS_{zz}}{dt} = \frac{4}{3}G\left(\frac{d\varepsilon_{zz}}{dt} + \frac{dW_{zz}}{dt}\right) - 2G\frac{dw_{zz}}{dt}, \tag{8}$$

$$\frac{dW_{zz}}{dt} = -\frac{1}{(1-\eta)}\frac{d\eta}{dt}, \tag{9}$$

$$\eta = n \cdot \left(2\pi R^3 \frac{\sigma_{zz}}{G}\right), \tag{10}$$

where $w_{zz}$ is the plastic distortion due to the dislocations movement; $U$ is the specific internal energy, $P$ is the pressure; $S_{zz}$ is deviator of stresses. All variables here are averaged over physically small volumes. The Eqs (5)-(10) have to be completed by the Eq. (1) and Eq. (3) for the

micro-cracks nucleation and growth and by the equations for determination of the plastic distortion $w_{ik}$ through the dislocations movement (see, for example, [17]). For determination of the pressure and temperature, the wide-range equations of state [18,19] were used in the forms of dependences $P = P(\rho, U)$ and $T = T(\rho, U)$. All equations have been integrated in time by the explicit Euler scheme with variable time step, which has been selected from the stability condition $\Delta t \le \min\{0.1R/\dot{R}; 0.001/\dot{\varepsilon}_{zz}\}$. Parameters $\gamma$ and $\Delta\gamma$ had been chosen by fitting with the experimental data [1-4,20-26] and with the of molecular-dynamics (MD) simulation results [7,9,10] for the strain rate dependences of the material strength; the obtained values of these parameters are summarized in the Table 1.

Table 1. Parameters of the fracture model. Abbreviations: m/c – monocrystalline, p/c – polycrystalline.

| Substance | Cu | | Al | | Ti | Fe | Zn | Mo | |
|---|---|---|---|---|---|---|---|---|---|
| | m/c | p/c | m/c | p/c | p/c | p/c | m/c | m/c | p/c |
| $\gamma$, J/m$^2$ | 0.95 | 0.60 | 0.57 | 0.47 | 1 | 1 | 0.8 | 1.1 | 0.7 |
| $\Delta\gamma$, J/m$^2$ | 0.029 | 0.029 | 0.016 | 0.016 | 0.027 | 0.036 | 0.029 | 0.034 | 0.034 |

## 3. Results and discussion

Strain dependences of tensile stress have been obtained in calculations; the typical dependences are shown in Fig. 2(a). Stress grows up with strain at the initial stage. Then the tension reaches some critical level, an intensive nucleation and growth of the cracks begins. It leads to relaxation of tensile stresses; the increase of stresses is changed on the decrease. Non-zero level of tensile stresses is held till the complete destruction of substance. The moment of complete destruction corresponds to the slump of stresses down to zero. The maximal obtained value of tensile stresses has to be treated as the dynamic (spall) strength of the material $\sigma_{sp}$. Dynamic strength increases with the strain rate, because the growth rate of the total volume of cracks has to be proportional to the strain rate for effective relaxation of the tensile stresses. This total volume is determined by the number and size of cracks; therefore, nucleation and growth rates have to be increased for relaxation at the increased strain rate, these rates are obtained at higher level of the tensile stresses.

Fig. 2(b) shows the strain dependences of the average radius $R$, the critical radius $R_{cr}$ and the concentration $n$ of the micro-cracks. Nucleation of cracks starts at the earliest stages of deformation, but its concentration is insignificant initially. At the low acting stresses, voids are nucleated only in weakened zones with a very high value of faultiness $\gamma^* \approx \gamma$, concentration of which is negligibly small. The critical radius decreases with the increase of strains and of the tensile stresses; zones with lower faultiness begin to contribute in nucleation of cracks, and the concentration of cracks grows fast. When the concentration reaches some value, the relaxation on micro-cracks becomes a dominant process, and the tensile stresses begin to decrease (see Fig. 2 (a)). It initiates an increase of the critical radius and slump of the nucleation rate of new cracks, only the growth of the existing micro-cracks takes place. This growth continues up to the reaching of the complete destruction, after than, $R$ means a typical size of fragments in the destructed material. It is 30 μm and 7 μm for the strain rates $10^6$ s$^{-1}$ and $10^7$ s$^{-1}$ correspondently.

The calculated strain rate dependencies of the dynamic strength for monocrystalline and polycrystalline copper and aluminum are presented in Fig. 3 in comparison with the experimental data and MD simulation results. The model parameters $\gamma$ and $\Delta\gamma$ (Table 1) have been chosen for

fitting our results with experiments and MD modeling. At the same time, the fracture model gives correct slopes of the curve $\sigma_{sp}\left(d\varepsilon/dt\right)$ in the both regimes of nucleation, and these slopes are not regulated by the model parameters. For unequivocal selecting of the parameters a simultaneous comparison with experimental data at the moderate strain rates (heterogeneous nucleation) and with results of MD simulations at very high strain rates (homogeneous nucleation) is optimal.

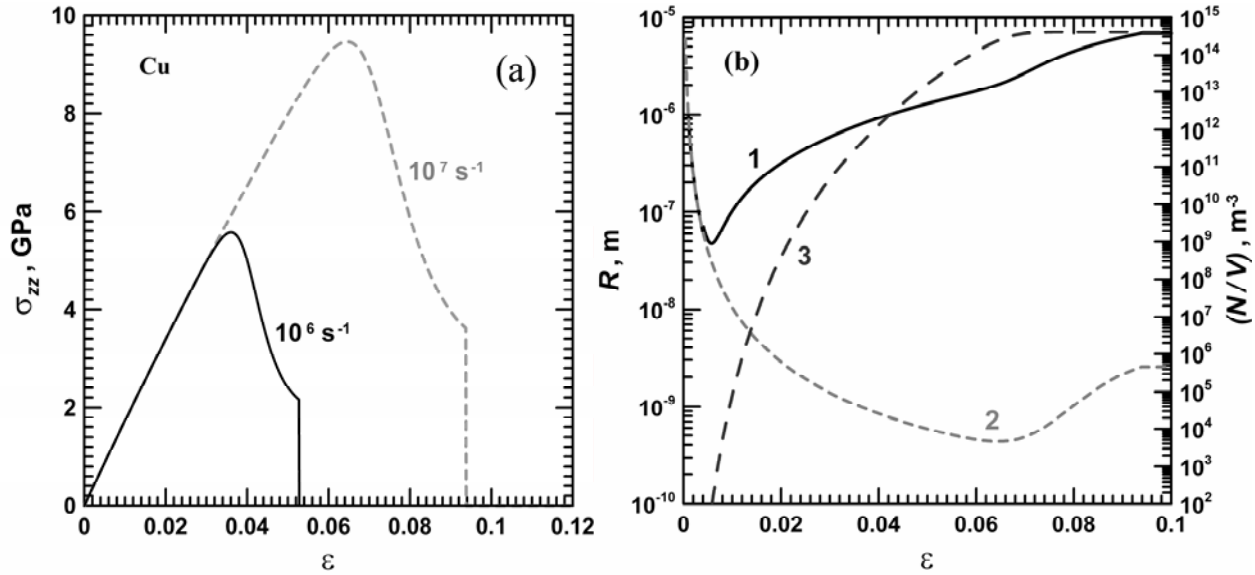


Figure 2. The strain dependence of stresses at two constant strain rates in the monocrystalline copper (a). Strain dependences of the average micro-cracks radius (1), the critical radius (2) and the concentration of micro-cracks (3) at the constant strain rate и $10^7$ s$^{-1}$ (b).

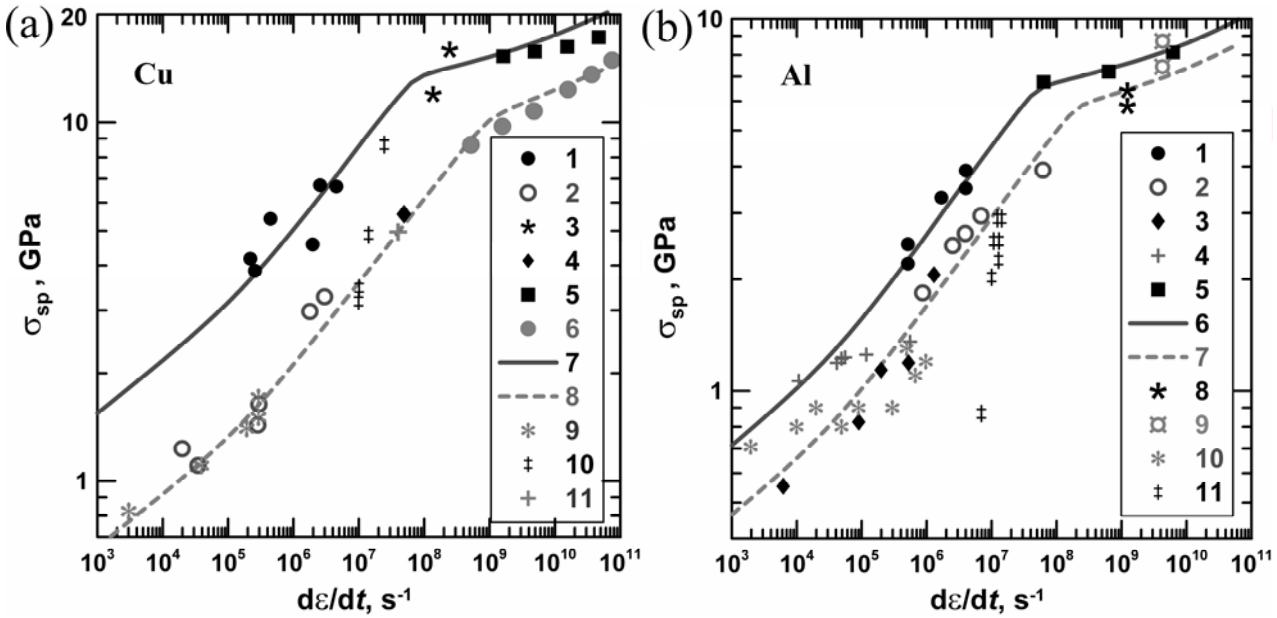


Figure 3. The strain rate dependences of the dynamic strength of copper (a) and aluminum (b). For copper (a): experimental data for monocrystals 1 – [2] and 3 – [20]; experimental data for polycrystals 2 – [2], 4 – [21], 9 – [22], 10 – [4], 11 – [23]; markers 5 for monocrystal and 6 for polycrystal are the results of MD [7]; lines are predictions of the model for monocrystals 7 and polycrystals 8. For aluminum (b): experimental data, 1 - monocrystal [1], 2 - polycrystal of 99.9% purity [24], 3 – alloy AlMg6 [25], 4 - commercially pure aluminum AD1 [26], 8 – polycristals [3], 10 – [22], 11 – [4]; results of MD for monocrystals (5) - [10] and 9 - [9]; lines are predictions of the model for monocrystals 6 and polycrystals 7.

Experimental results at the strain rates $\leq 10^8$ s$^{-1}$ correspond to the regime of heterogeneous nucleation then the formation of micro-cracks occurs on inhomogeneities (defects of the exponential spectrum). MD results and experiments [3,20] for the strain rates $>10^8$ s$^{-1}$ correspond to the mode of homogeneous nucleation when the micro-cracks are typically formed in homogeneous parts of material (zones of perfect crystal or zones with a bundle of identical defects). The term «homogeneous nucleation» is conditional for polycrystals because in this case the fracture begins in the grain boundaries [7]. Therefore, we use here this term in the sense of presence of a quantity of identical uniformly distributed defects, for example, grain boundaries (in contrast with the defects of exponential spectrum).

Calculations show, that plasticity is a dominant factor influencing on the voids growth and on the dynamic strength at the strain rates $\leq 10^4$ s$^{-1}$. On the contrary, at the strain rates $\geq 10^7$ s$^{-1}$, the plasticity is negligible in the dynamic strength calculations, but it can influences on the resulting form of voids and on the picture of destructed material.

## 4. Conclusions

The micro-cracks nucleation and growth have been analyzed for the purpose of the dynamical fracture description. The model was formulated, which agrees well with experimental and MD data on the strain rate dependence of the dynamic strength for a number of metals. This model can be practically used in the material dynamics simulations. The strain rate dependence of the dynamic strength has two different regions corresponding to regimes of the heterogeneous nucleation (at the strain rates $< 10^8$ s$^{-1}$) and the homogeneous nucleation (at the strain rates $> 10^8$ s$^{-1}$). In the first case, the weakened zones of the material play an important role in fracture. In the second mode, the number of weakened zones is insufficient, voids are nucleated in undefected material, and the strength growth is decelerated. It contradicts with the commonly used uniform power dependence of $\sigma_{sp}$ on $d\varepsilon/dt$ [3,10] in the whole region of the strain rate, therefore, the ideal strength [3] can be achieved at the higher strain rates (above $10^{11}$–$10^{12}$ s$^{-1}$), than it follows from the power dependence.

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