# Numerical simulation of plasticity and failure of solids with defects under dynamic loading

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**Abstract.** The developed statistical model of solid with mesoscopic defects allowed the formulation of phenomenological model in terms of two independent variables – the defect density tensor and structural scaling parameter and the simulation of shock wave propagation in the linkage with structural relaxation phenomena [1-5]. It was established the link of non-linearity of plasticity and failure and the kinetics of structural scaling transition in the metastability area of out-of-equilibrium thermodynamic potential of solid with mesodefects with application to the analysis of spall failure. The purpose of the present work consists of development of three-dimensional mathematical model of solid with defects and the further verification of model. According the decomposition of stress and strain tensors on isotropic and deviatoric parts the kinetic equations for respective parts of defect density tensor were introduced. The deviatoric part evolution corresponds to mechanisms of plastic relaxation and isotropic part evolution corresponds to microcrack growth and failure.

Developed constitutive equations of solids with mesoscopic defects were implemented into commercial numerical codes (Abaqus/Explicit).

## Introduction

Deformation and failure under intensive loading are linking to the defect induced relaxation process that has qualitative different scenarios depending on the initial structure and strain rates. Structure induced relaxation properties and failure are related to the multiscale dislocation evolution that include the stages of new dislocation substructure nucleation and growth in the presence of external stress and due to interaction with other dislocation and dislocation substructures (mesodefects). The statistical model of solid with mesodefects [1-7] that is operated with internal variables, the defect density tensor, characterizing the mesodefect induced strain and an additional variable – the structural-scaling parameter, which reflects the spatial scale evolution in mesodefects ensembles – the scale of corresponding dislocation substructures and the spacing between them.

The influence of mesodefects on the relaxation properties and damage-failure transition was described in the framework of statistically based phenomenological approach that reflects specific types of nonlinear behavior of the out-of-equilibrium systems “ solid with mesodefects” called as structural-scaling transition [1].

The purpose of this work is the adaptation of mentioned model to the impact loading and the following verification of material parameters using the data of plate impact test for the vanadium (pull-back velocity measurement after VISAR).

## Mathematical statement

Mathematical statement of moderate shock wave front propagation in sold with defects is analyzed. Constitutive modeling follows to results given by the statistical theory of collective behavior of defects and for the conditions of the plate impact test is formulated for the component of the strain rate $\varepsilon_{xx} \neq 0$ (others components of the strain tensor equal zero).

Plasticity mechanisms are linked to the structural variables (defect density tensor and structural scaling parameter) and corresponding collective modes that reflect the collective behavior of defects.

Defect density tensor $\tilde{p} = n\langle \tilde{s} \rangle$ is associated with the defect induced strain in the specific volume, where $\tilde{s}$ is microscopic tensor related to the geometrical strain induced by microcrack or microshear; $n$ is the microcrack (microshear) density. Defect evolution is characterized by the defect nucleation, defect growth and the motion of defects in the condition of the interactions of defects in the presence of structural and applied stresses.

These mechanisms give the corresponding part in the total strain (or strain rate) that represents the visco-elastic plastic flow:

$$\dot{\tilde{\varepsilon}} = \dot{\tilde{\varepsilon}}^{e} + \dot{\tilde{p}} + \dot{\tilde{\varepsilon}}^{p} \tag{1}$$

where $\dot{\tilde{\varepsilon}}^{e}$ is the elastic strain rate, $\dot{\tilde{p}}$ is the geometrical defect induced strain rate, $\dot{\tilde{\varepsilon}}^{p}$ is the viscous plastic strain rate. Statistical model allowed the formulation of thermodynamic potential (non-equilibrium free energy $F$) and the definition of the part of the dissipation function related to defects:

$$T\dot{S} = \tilde{\sigma} \cdot\cdot \dot{\tilde{\varepsilon}}^{p} + \left(-\frac{\partial F}{\partial \tilde{p}}\right) \cdot\cdot \dot{\tilde{p}} + \left(-\frac{\partial F}{\partial \delta}\right)\dot{\delta} \geq 0 \tag{2}$$

where $S$ is the entropy, $T$ is the temperature.

To follow the Onsager principle the constitutive relations of visco-elastic plastic solid can be written as the link of thermodynamic forces and thermodynamic fluxes:

$$\begin{aligned}
&\tilde{\sigma} = A_1 \dot{\tilde{\varepsilon}}^{p} - A_2 \dot{\tilde{p}},\\
&-\frac{\partial F}{\partial \tilde{p}} = A_3 \dot{\tilde{p}} - A_2 \dot{\tilde{\varepsilon}}^{p},\\
&-\frac{\partial F}{\partial \delta} = A_4 \dot{\delta},\\
&A_1 A_3 - A_2^2 \geq 0\\
&A_i > 0, i = \overline{1,4}
\end{aligned} \tag{3}$$

where $A_1, A_2, A_3, A_4$ are the kinetic coefficients that depend in general case on thermodynamic variables $\tilde{p}$, $\delta$ and temperature.

Using the equations $(3)_1$ and $(3)_2$, the kinetics of plastic deformation can be determined as

$$\dot{\tilde{\varepsilon}}^{p} = \left( \frac{A_3}{A_1 A_3 - A_2^2} + \frac{A_2}{A_1 A_3 - A_2^2} \frac{\left(-\frac{\partial F}{\partial \tilde{p}}\right)}{\tilde{\sigma}_d} \right) \tilde{\sigma}_d \tag{4}$$

where the expression in the bracket has the meaning of the inverse effective viscosity; $\tilde{\sigma}_d$ is the deviatoric part of stress. As it follows from the effective viscosity presentation the visco-plastic response of material depends on the current structural state induced by defects and applied stress

$$\dot{\tilde{\varepsilon}}^p = \frac{1}{\tau_s(\tilde{p},\tilde{\sigma}_d)}\tilde{\sigma}_d \tag{5}$$

Taking into account $(3)_2$ and (4) the kinetics for the defect density tensor reads:

$$\dot{\tilde{p}} = \frac{A_2}{A_1A_3 - A_2^2}\tilde{\sigma}_d + \frac{A_1}{A_1A_3 - A_2^2}\left(-\frac{\partial F}{\partial \tilde{p}}\right) \tag{6}$$

where two mechanisms responsible for the damage evolution are presented: initiation of defect nuclei due to the viscous plastic flow and the defect growth due to the free energy release. Similar (5) Eqn. (6) can be written in the form

$$\dot{\tilde{p}} = \frac{1}{\tau_p(\tilde{p},\tilde{\sigma}_d)}\left(-\frac{\partial F}{\partial \tilde{p}}\right) \tag{7}$$

where $\tau_p(\tilde{p},\tilde{\sigma}_d)$ is the characteristic time for the damage evolution. The system of equations for plastic strain rate $\dot{\tilde{\varepsilon}}^p$ and thermodynamic variables $\tilde{p}$, $\delta$ can be presented in the unified form

$$\begin{aligned}
\dot{\tilde{\varepsilon}}^p &= \frac{1}{\tau_s(\tilde{\sigma}_d)}\tilde{\sigma}_d \\
\dot{\tilde{p}} &= \frac{1}{\tau_p(\tilde{\sigma}_d)}\left(-\frac{\partial F}{\partial \tilde{p}}\right) \\
\dot{\delta} &= \frac{1}{\tau_\delta}\left(-\frac{\partial F}{\partial \delta}\right)
\end{aligned} \tag{8}$$

Motion equation reads

$$\nabla \cdot \tilde{\sigma} = \rho \ddot{\vec{u}} \tag{9}$$

where $\tilde{\sigma}$ is the tensor of total stress, $\rho$ is the density, $\vec{u}$ is the displacement.

The total stress represents the sum of deviatoric $\tilde{\sigma}_d$ and isotropic $\tilde{\sigma}_o$ parts:

$$\tilde{\sigma} = \tilde{\sigma}_d + \tilde{\sigma}_o. \tag{10}$$

Using the rate version of the Hook low

$$\dot{\tilde{\sigma}} = \lambda I_1(\dot{\tilde{\varepsilon}}^e) + 2G\dot{\tilde{\varepsilon}}^e \tag{11}$$

where $\lambda$ is the Lame coefficient, $G$ is the elasticity modulus, $I_1(\tilde{x})$ is the first invariant of tensor $\tilde{x}$, $\tilde{\varepsilon}^e$ is the elastic strain. The components $\dot{\sigma}_o$ and $\dot{\sigma}_d$ for the uni-axial case corresponding to the plate impact test read

$$\begin{aligned}
&\dot{\sigma}_d = 2G\left(\frac{2}{3}\dot{\varepsilon} - \dot{p} - \dot{\varepsilon}^p\right),\\
&\dot{\sigma}_o = K\dot{\varepsilon},
\end{aligned} \tag{12}$$

where $K$ is the bulk modulus.

Motion equation (9) for the plate impact condition can be represented in the form:

$$\frac{\partial^2 \sigma}{\partial x^2} = \rho \frac{\partial \dot{\varepsilon}}{\partial t}, \tag{13}$$

where $\dot{\varepsilon} = \dfrac{\partial V}{\partial x}$, $V$ is the velocity.

Taking into account the constitutive equations providing the link of relaxation mechanisms and defect induced structural-scaling transitions the system of dimensionless equations can be written:

$$\begin{aligned}
&\frac{\partial \Sigma_d}{\partial \tau} = -\frac{\partial \eta}{\partial \tau} - \frac{\partial \varepsilon^p}{\partial \tau} + \frac{2}{3}\beta,\\
&\frac{\partial \Sigma_o}{\partial \tau} = \frac{(1+\nu)}{3(1-2\nu)}\beta,\\
&\Sigma = \Sigma_d + \Sigma_o,\\
&\frac{\partial \eta}{\partial \tau} = \chi \frac{\partial^2 \eta}{\partial \xi^2} + \Gamma_p\left(-\frac{\partial \Psi}{\partial \eta}\right),\\
&\frac{\partial \beta}{\partial \tau} = \frac{\partial^2 \Sigma}{\partial \xi^2},\\
&\frac{\partial \delta}{\partial \tau} = \Gamma_\delta\left(-\frac{\partial \Psi}{\partial \delta}\right),\\
&\frac{\partial \varepsilon^p}{\partial \tau} = \Gamma_\sigma \Sigma_d,\\
&\Gamma_i = \frac{\tau_H}{\tau_i}, \tau_i = \tau_{io}\exp\left(-\frac{|\Sigma_d|}{\sigma_c}\right), i = p, \sigma \qquad \Sigma_d\big|_{\tau=0} = 0, \Sigma_d\big|_{\xi=0} = 0, \Sigma_d\big|_{\xi=1} = 0\\
&\Gamma_\delta = \frac{\tau_H}{\tau_\delta}, \tau_\delta = const \qquad \Sigma_o\big|_{\tau=0} = 0, \Sigma_o\big|_{\xi=0} = \sigma_{input}(\tau), \Sigma_o\big|_{\xi=1} = 0\\
&\sigma = 2G\Sigma, x = h\xi, t = \frac{h}{C_l}\tau, V = C_l v, \qquad \eta\big|_{\tau=0} = 0, \left.\frac{\partial \eta}{\partial \xi}\right|_{\xi=0,\xi=1} = 0\\
&F = F_m \Psi \qquad \beta\big|_{\tau=0} = 0, \delta\big|_{\tau=0} = \delta_0, \varepsilon^p\big|_{\tau=0} = 0
\end{aligned} \tag{15}$$

where $E^p$ is the plastic strain, $\Gamma_\sigma, \Gamma_\delta, \Gamma_p, \chi$ are the kinetic coefficient, $\Psi$ is the non-equilibrium free energy, $\Sigma_d$ is the deviatoric part of stress, $\Sigma_o$ is the isotropic part of stress, $\eta$ is the geometrical defect induced strain, $\tau$ is the time, $\xi$ is the coordinate, $\sigma_{input}(\tau)$ is the input stress pulse, $\Delta$ is structural-scaling parameter, $\beta = \frac{\partial E}{\partial \tau}$ is the intermediate variable that allowed reformulation of equation from the hyperbolic to the parabolic form, $E$ is the total strain, $C_l$ is the longitudinal sound speed, $h$ is the width of plate, $\nu$ is the Poison coefficient.

The kinetic coefficients $\tau_i \quad (i = p, s, \delta)$ determine the relaxation properties of materials: $\tau_p$ is the characteristic time of orientation ordering and growth of defects, $\tau_\delta$ is the characteristic time of scaling transition in defects ensemble; $\tau_s$ is the relaxation time of the stress induced transition.

**Numerical results**

The system of equations (15) was solved numerically using finite difference explicit scheme. The parameters of model were identified using the original optimization method based on the minimization procedure of square deviation of experimental and numerical curves corresponding to quasi-static and dynamic tests [8]. Numerical plot for plat impact loading is presented in Fig. 6 in the comparison with experimental data [9].

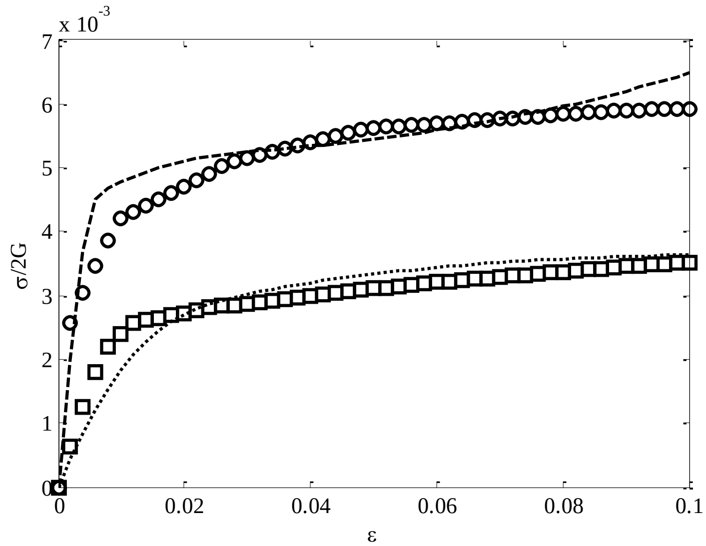



Fig. 1. Experimental and numerical stress-strain curves for the strain rates $10^{-1}$ $s^{-1}$ (dotted curve) and $10^3$ $s^{-1}$ (stripped curve): numerical results mark by symbols ($10^{-1}$ $s^{-1}$– □, $10^3$ $s^{-1}$– ○).

The following values of kinetic coefficients and parameters of model were estimated: $\tau_{po} = 0.276$ s, $\tau_{so} = 2.22$ s, $\tau_{\delta o} = 296.5$ s, $\delta_o = 1.96$, $p_c = 0.0228$, $\sigma_c = 0.0009$.

Results of numerical simulation of the plate impact test and the comparison of the pull-back velocity (symbol ○ for the modeling) with experimental data (solid line) from the VISAR technique [9] are presented in Fig. 2.

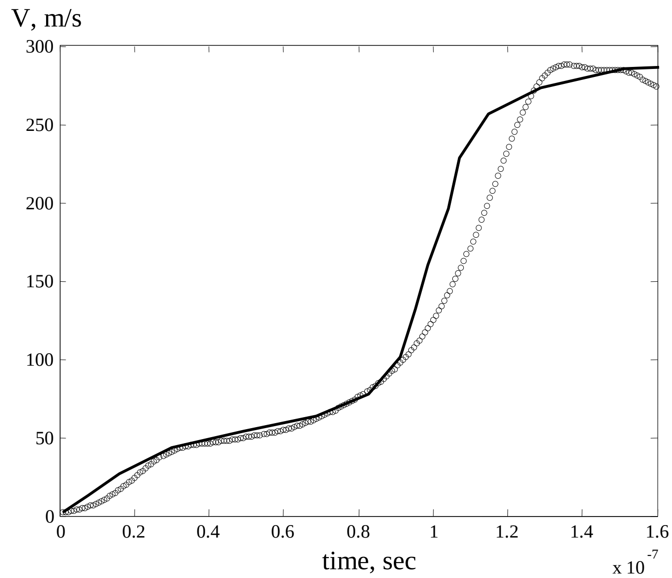



Fig. 2. Free surface particle velocity of vanadium target with the thickness 5047 mm

Two-wave configuration was found after experiment that corresponds to the stability loss of the shock wave and the transition from the elastic to plastic deformation (flow). The modeling of shock wave loading of vanadium target was combined with the simulation of damage-failure transition in the rarefaction wave and spall failure initiation.

The damage-failure transition was described as the development of blow-up kinetics of damage accumulation. To avoid the numerical problems related to the blow-up damage kinetics the following criteria was introduced

$$|\eta||\nabla\eta| \geq H_c \tag{17}$$

where $H_c$ is the critical value that defines the failure occurring on some characteristic scale related to the scale of the blow-up dissipative structure. Particle velocity profiles are presented in Fig. 3 for vanadium targets. The correspondence of numerical results and experimental data allowed the conclusion that mentioned criteria can be used for the estimation of spall failure initiation under intensive loading.

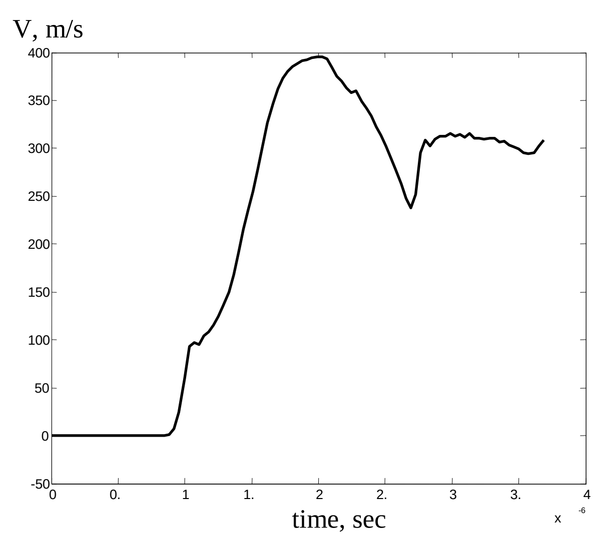
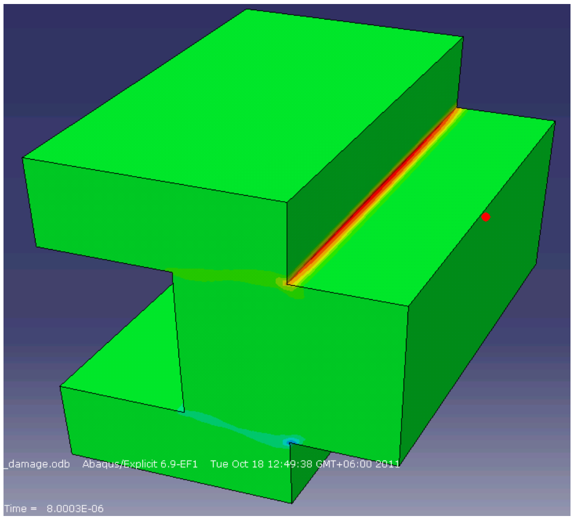
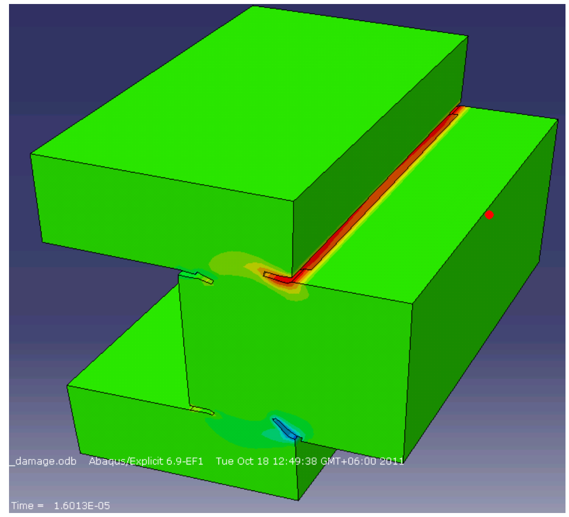



Fig. 3. Numerical simulation results of spall failure in vanadium

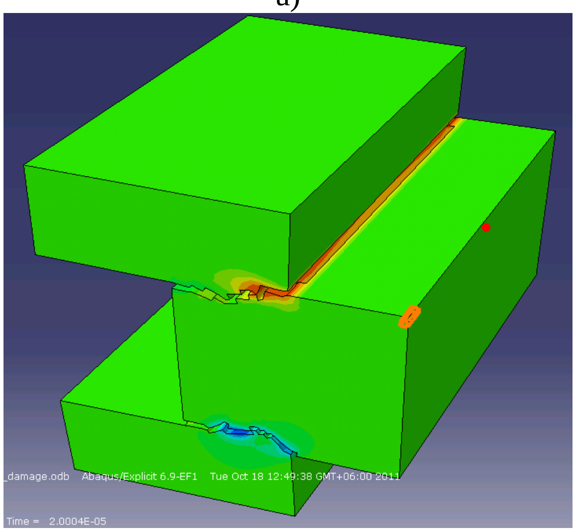
The equations (8-11) for three-dimention case were implemented into the comercial FEM code (Abaqus/Explicit). Dynamic shear loading of vanadium scecimens was considered. Three-dimention numerical simulation results of dynamic shear loading and failure are presented in Fig. 4 for different times. Presented results show the acumulations of defects in terms of mention structural strain induced by defects in shear zones and folowing failure according to the estimated criteria (17).



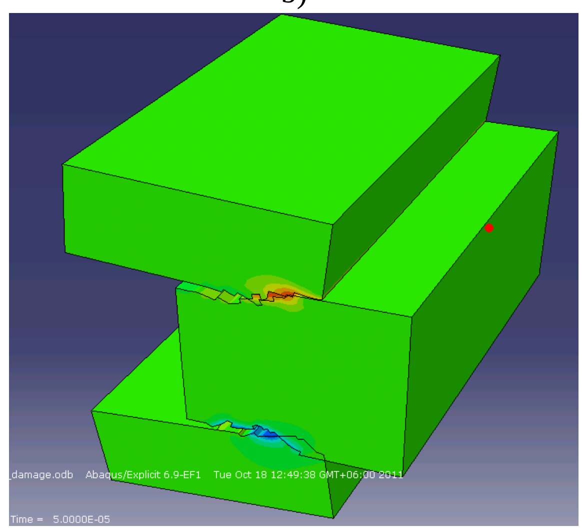

a)




b)




c)




d)

Fig. 4. Distribution of structural strain of defects and failure for dynamic shear loading using Hopkinson bar tests (numerical results, a – 8 μs, b – 16 μs, c – 20 μs, d – 50 μs)

**Summary**

Study of the shock wave profiles provides the important information concerning elastic, visco-plastic properties, the strength of materials subject to the shock wave loading. Comparative analysis of experimental and theoretical profiles showed that statistically based model allowed the description of relaxation properties and damage-failure transition in the large range of load intensities using two internal variables that are responsible for the multiscale evolution of defects. Kinetics of these internal variables illustrates the linkage of characteristic stages of defects evolution, relaxation ability of materials, damage accumulation stages under the spall failure initiation.

The model constants were identified according to the stress-strain diagrams of dynamic loading (Hopkinson bar tests) at different strain rates. Model verification was based on the plate impact experiments. Procedure of identification and verification of developed model was carried out for wide range of strain rates (quasistatic, dynamic and shock loading) for vanadium [6,7]. In the present work numerical results of three-dimensional dynamic experiments of plate impact and pure shear experiments are presented. The obtained results correspond to experimental data very precisely.

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