Numerical simulation of multiscale damage-failure transition and shock wave propagation in metals and ceramics

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Abstract. Statistical theory of evolution of typical mesoscopic defects revealed specific type of criticality - structural-scaling transitions and allowed the development of phenomenology of damage and plastic flow in materials under intensive loading, which established characteristic multiscale collective modes of defects responsible for formation of plastic waves and damage-failure transition. Original approach based on wide range constitutive equations was developed for simulation of multiscale damage-failure transition mechanisms and shock wave propagation in metals and ceramics in range of strain rate $10^3 - 10^8 \text{ s}^{-1}$. It was shown that mechanisms of a plastic relaxation and damage-failure transitions are linked to multiscale kinetics of mesodefects collective modes with the nature of solitary waves and blow-up dissipative structures consequently. Numerical simulation of original plate impact tests showed that the model describes shock wave loading for metals and ceramics, and allowed us to explain the effect of power law phenomena of plastic wave fronts formation, its self-similar features under reloading and unloading. Analysis of shock wave profiles in ceramics for different thicknesses of specimens in terms of self-similar variables supports the universality of shock wave fronts.

1. Introduction
Recent investigations of the materials behavior under extreme loading conditions in plate impact test are of the great interest. It is associated with the wide range of applications based on effects of shock waves propagation in solids. During last decades the great number of materials, usually metals, were investigated under plate impact tests. One of the most important materials characteristics is the capacity to resist failure by tensile stresses. Macroscopic plastic strain distribution in material under impact loading defined by mechanical properties, which depends on temperature, loading rate, the deformation history and other factors. Mesoscopic defects occur in the materials during deformation, and lead to failure processes in matter and fracture. Thus, the deformation and fracture associated with the defects evolution. These processes are connected and can be considered as different demonstrations of the structural relaxation mechanisms, which are macroscopic manifestations of plastic flow and fracture.

The basis of most modern behavior of metals models under different loading conditions is the theory of the defect structure evolution. In this paper simulation of dynamic deformation is based on the structural-kinetic model on basis of the statistical-thermodynamic approach [1 - 3]. This approach takes into account kinetics of mesoscopic defects nucleation and growth. The
model describes the various stages in the defects evolution: particular accumulation mesoscopic defects, localized damage, as specific mechanisms of relaxation properties of material. This approach was described in terms of independent thermo-dynamic variables - defect induced strain and structural scaling parameter associated with two characteristic structural scales (the mesodefect nucleus radius and the distance between defects).

2. Numerical simulation

Mathematical statement was formulated in term of plan shock wave loading. In [4] the mathematical model of behavior of metals under shock-wave loading was developed. Identification of model parameters were carried out for aluminum, vanadium and iron using optimization described procedure in [5].

Initial system of differential equation consist of balance equations and constitutive relation that are presented below. Equation of motion and constitutive equations have form

\[ \nabla \cdot \tilde{\sigma} = \rho \ddot{u} \]  
(1)

\[ \frac{1}{\rho} \frac{dp}{dt} = -\nabla \cdot \tilde{v} \]  
(2)

\[ \dot{\varepsilon} = \dot{\varepsilon}^e + \dot{p} + \dot{\varepsilon}^p \]  
(3)

\[ \ddot{\sigma} = A_1 \dot{\varepsilon}^p - A_2 \dot{p} \]  
(4)

\[ \ddot{p} = \frac{A_2}{A_3} \dot{\varepsilon}^p - \frac{1}{A_4} \frac{\partial F}{\partial p} \]  
(5)

\[ \dot{\delta} = -\frac{1}{A_4} \frac{\partial F}{\partial \delta} \]  
(6)

\[ A_1 A_3 - A_2^2 > 0, A_i > 0, i = 1,4 \]  
(8)

where \( \tilde{\sigma} \) - stress, \( \rho \) - density, \( \ddot{u} \) - translation. Total strain \( \dot{\varepsilon} \) in the framework of proposed model consists of reversible and irreversible parts. Where reversible part is elastic deformation \( \dot{\varepsilon}^e \), irreversible by-turn is divided into nondissipative (defect induced strain \( \dot{p} \)) and dissipative (plastic \( \dot{\varepsilon}^p \)) parts. This separation allowed recording additive law (3). Hooke’s law was used in form (4), where \( \lambda \) and \( G \) - first and second Lame’s parameters, \( I_1(\dot{\varepsilon}^e) \) - first invariant of elastic deformation rate. Association of thermo-dynamics forces and fluxes was formulated according to Onsager principle (5-7), where \( F \) - Helmholtz energy, \( \delta \) - structural scaling parameter, \( A_i, i = 1,4 \) - kinetic coefficients [1-3].

Expression for the stress and defect induced strain were noted with regard for the different influence isotropic (index \( s \)) and deviatoric (index \( d \)) parts:

\[ \tilde{\sigma} = \tilde{\sigma}_s + \tilde{\sigma}_d \]  
(9)

\[ \tilde{p} = \tilde{p}_s + \tilde{p}_d \]  
(10)

Boundary conditions for one-dimension case (\( \varepsilon_{xx} \neq 0 \)) are given in the following form:

\[ \tilde{\sigma}_s \big|_{t=0} = 0, \]  
\[ \tilde{\sigma} \big|_{t=0} = 0, \tilde{\sigma} \big|_{x=0} = \sigma_{input}(t), \tilde{\sigma} \big|_{x=1} = 0, \]  
\[ \tilde{p}_s \big|_{t=0} = 0, \tilde{p}_d \big|_{t=0} = \tilde{p}_d \big|_{t=0} = 0, \]  
\[ \varepsilon^p \big|_{t=0} = 0, \]  
\[ \dot{\delta} \big|_{t=0} = \delta_{d0}, \dot{\delta} \big|_{t=0} = \delta_{s0}, \]  
\[ \rho \big|_{t=0} = \rho_0, v \big|_{t=0} = 0. \]  
(11)
3. Results

The system (1)-(10) for one-dimension case ($\varepsilon_{xx} \neq 0$) with boundary conditions (11) was solved numerically using finite difference explicit scheme. According numerical simulation results the profiles of free surface velocity for ceramics was built in comparison of experimental data.

In [6] the experimental study was carried out for shock wave propagation in silicon carbide with different thickness of samples. Free surface velocity profiles are presented on figure 1 for the sample thickness 2.15, 3.81, 8.32 mm and flyer thickness 2 mm with velocity 1.8 km/s. Figure 1 contains normalized wave profiles for different thickness specimens ($h$). These results demonstrated the self-similarity of shock wave fronts in ceramics. Numerical simulation of shock wave loading for ceramic (silicon carbide) allowed us to obtain a satisfactory agreement with experimental data.

The system (1)-(10) was numerically solved for shock wave loading of vanadium. The response for vanadium under plane impact test is different from ceramics. The recorded shock wave profiles show separation on elastic precursor and plastic front (figure 2). In the present work the simulation of spall fracture of metals carried out. This type of failure was considered in terms of nucleation and growth of volume type defects. Spall failure is determined by the location of the blow-up damage localization kinetics [1, 2]. One of the most important mechanical property of material is spall strength. It is well known that load intensification leads to the spall strength increasing. According to the obtained profiles of free-surface velocity the spall strength of vanadium was determined for different strain rates (figure 3). In [8-9] the experimental study shock wave loading for vanadium was carried out. Comparison of our results allows us to conclude that the developed mathematical model adequately describes experimental data [9] (figure 4).

4. Conclusions

The behavior of metals [3-4] and ceramics [5] under shock wave loading was numerically simulated. Response of materials on the dynamic loading confirms to experimental data [6]. Obtained results show that developed model [4] described shock wave loading for ceramics and metals. Analysis of shock wave profiles for different thicknesses of specimens shows the self-
Figure 3. Free surface velocity profiles in vanadium specimen for different loads.

Figure 4. Spall strength vs strain rate for vanadium, square - experimental data [9], circle - numerical result.

similarity of shock wave fronts in terms of special autombel variables - free surface velocity versus time divided by thickness of specimen.

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