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MULTISCALE MODELS OF PLASTICITY AND TENSILE FRACTURE OF METALS AT HIGH-RATE DEFORMATION

ALEXANDER E. MAYER, VASILIY S. KRASNIKOV AND VICTOR V. POGORELKO

Department of Physics
Chelyabinsk State University (CSU)
Bratiev Kashirinykh 129, 454001, Chelyabinsk, Russia
e-mail: mayer@csu.ru

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Summary. We describe our multi-scale approach for construction of the dynamic plastic deformation model and the tensile (spall) fracture model. The basic frameworks are briefly discussed and some of calculation results are shown.

1 INTRODUCTION

Modern experimental techniques allow one to get a wide range of strain rate up to an inverse nanosecond [1]. The commonly used empirical models of plasticity and fracture become unacceptable at this ultra-high-rate deformation. Moreover, there are a lot of evidences about the influence of initial microstructure on the mechanical behavior of materials at shock loading [2]. All this raises importance of the physically-based models [3] with an explicit accounting of structural defects (dislocations, voids) as elementary carriers of plasticity and fracture. These models can include more complicated equations with larger number of parameters in comparison with the empirical one, but the equations can be verified and parameters can be determined by means of the molecular dynamic (MD) simulations.

Here we report our models of the dynamic plastic deformation [3,4] and tensile fracture [5,6] of metals. The models are constructed in the following way: the atomistic simulations are used at the first stage for investigation of the dynamics and kinetics of the structural defects; equations of the defect evolution are constructed, verified, and their parameters are identified by means of comparison with the atomistic simulations. Thereafter, the defect evolution equations are incorporated into the continuum model of the substance behavior on the macroscopic scale. The obtained continuum models with accounting of defects subsystems are tested by comparison with the experimental results known from literature.

2 MATHEMATICAL MODEL

Continuum model supposes an averaged description of the lattice defects in the form of various parameter fields (scalar density of dislocations, concentration of voids, etc.).

2.1 Strains and stresses

The elastic deformation creating the shear stresses is defined as a difference between the geometrical deformation $\mathbf{u}$ determined by the macroscopic motion of substance

$$\dot{\mathbf{u}} = \mathrm{sym}(\nabla \cdot \mathbf{v}) \tag{1}$$

where $\mathbf{v}$ is the substance velocity, and the plastic deformation $\mathbf{w}$ determined by the microscopic motion of dislocations. The presence of voids leading to the spall fracture is taken into account by means of the fracture tensor $\mathbf{W}$ describing the mean deformation of the solid material due to the void growth; the trace of this tensor $W = \mathrm{trace}(\mathbf{W})$ enters the main equations. The complete stresses $\boldsymbol{\sigma}$ are divided on the spherical part $P = -\mathrm{trace}(\boldsymbol{\sigma})/3$ (pressure) and the deviatory stress $\mathbf{S}$: $\boldsymbol{\sigma} = -P \cdot \mathbf{I} + \mathbf{S}$, where $\mathbf{I}$ is the unit tensor. A wide-range equation of state is used for calculating the pressure P as a function of the density ρ and internal energy E, while the deviatory part is calculated with using a generalized Hook's law

$$\mathbf{S} = 2G\left(\mathbf{u} + \mathbf{W} - \mathbf{I} \cdot \mathrm{trace}(\mathbf{u} + \mathbf{W})/3 - \mathbf{w}\right) \tag{2}$$

where G is the shear modulus; $\mathrm{trace}(\mathbf{w}) = 0$.

2.2 Conservation laws

A standard set of the conservation equations is used with accounting of $\mathbf{w}$ and $\mathbf{W}$:

$$\dot{\rho} = -\rho\left[(\nabla \cdot \mathbf{v}) + \dot{W}\right] \tag{3}$$

$$\dot{\mathbf{v}} = \rho^{-1}\left[-(\nabla P) + (\nabla \cdot \mathbf{S}) - P(\nabla W) - (\mathbf{S} \cdot \nabla) W\right] \tag{4}$$

$$\dot{E} = \rho^{-1}\left[-P\left((\nabla \cdot \mathbf{v}) + \dot{W}\right) + (\mathbf{S} : \dot{\mathbf{w}})\right] + D \tag{5}$$

where D is the energy release function reflecting the action of irradiation if any.

2.3 Plasticity and fracture

The increase rate of the plastic deformation tensor $\mathbf{w}$ is calculated through the generalized Orowan's equation [3,4] using the values of the dislocation scalar density and velocity in each slip system. The atomistic simulations are useful for determination of the dislocation motion equation and its parameters [7,8]. The fracture tensor is calculated through the volume fraction of voids; atomistic simulations are used for fitting of the equations of voids nucleation and their subsequent growth [5,6].

4 RESULTS

Figure 1 presents the model verification for the high-velocity plate impact problem: comparison of the calculation results with the experimental data [9]. Figure 2 shows the 2D modeling of the stainless steel sample deformation and rear spallation under the action of the high-current electron beam (SINUS-7 accelerator [10]).

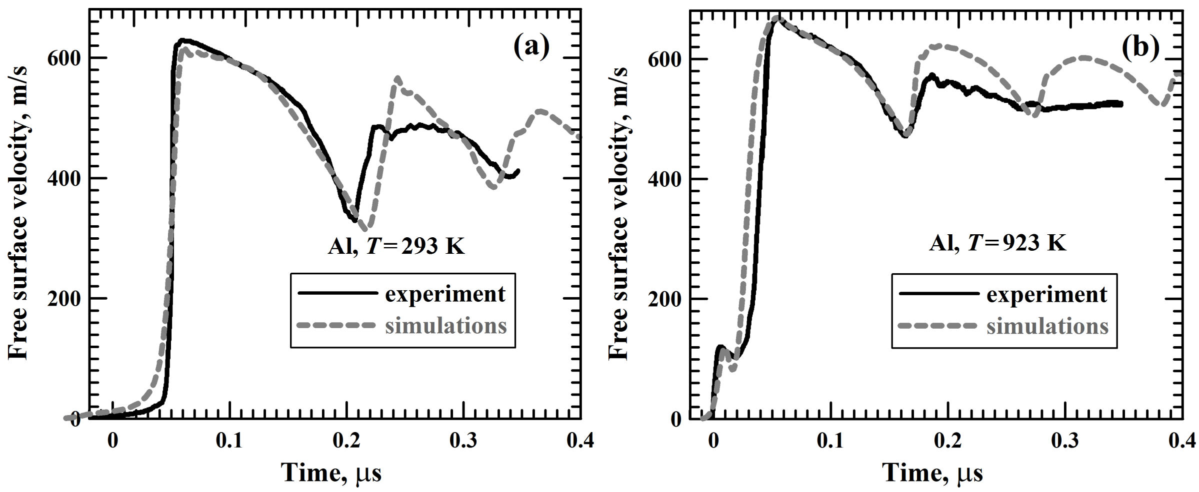

Figure 1: Verification of the models: back surface velocity histories for monocrysatlline aluminum at room (a) and elevated (b) temperatures. High-velocity impact with the impact velocity of 660 m/s ; thickness of the aluminum impactor is 0.4 mm ; the sample thickness is 2.9 mm. Comparison of the simulation results with the experimental data [9]. Shock wave with precursor and the following rarefaction wave with the spall pulse.

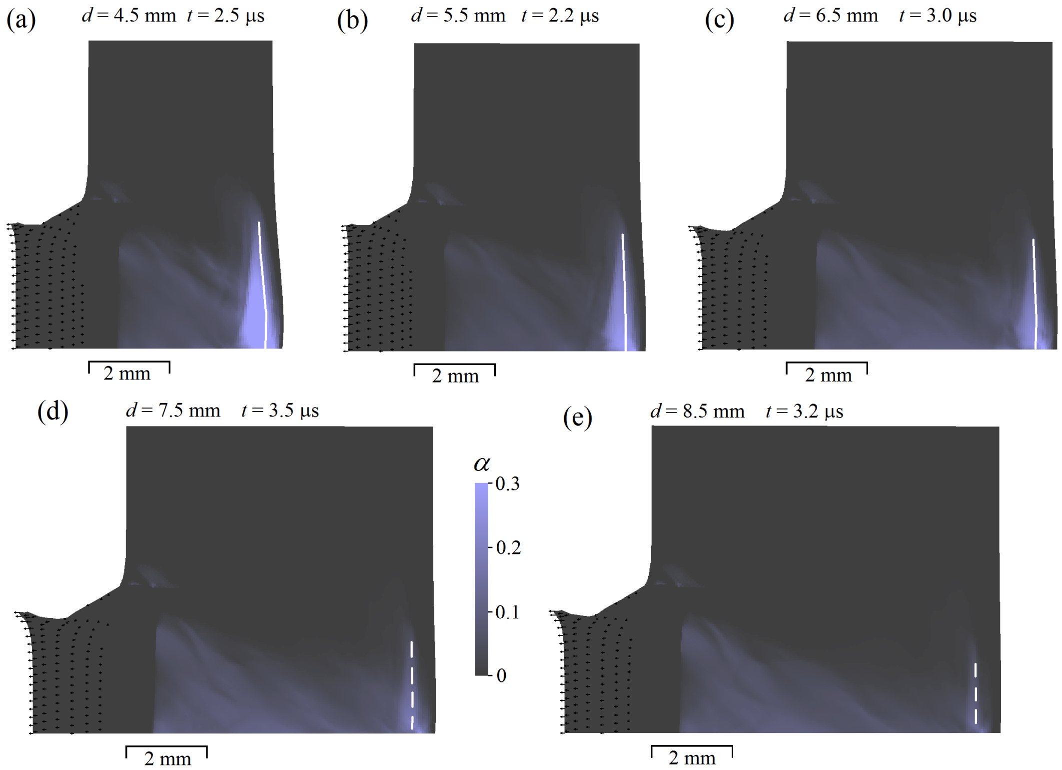

Figure 2: Calculated distributions of the volume fraction of voids α in samples with various thicknesses made of stainless steel and irradiated by the high-current electron beam (SINUS-7 accelerator [10]). (a,b,c) solid lines show the expected position of the main crack, (d,e) dashed lines show the expected position of the zone of incomplete fracture. Expanding cloud of ablated material is from the left. Little arrows on the left sides show the substance velocity vectors for the expanding ablated matter.

12 CONCLUSIONS

- Construction of the multiscale models of plasticity and fracture is in progress. They are based on the atomistic simulation of the elementary processes of the structural defect evolution, which are generalized in the form of continuum model applicable for the macroscopic deformation modeling in a wide range of parameters.

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