20th International Conference on Computer Methods in Mechanics

Short Papers

Editors:
T. Łodygowski
J. Rakowski
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Poznań 2013

Cover design
Anita Kaczor

ISBN 978-83-89333-51-3

Printed by:
A.R. COMPRINT
ul. Heleny Rzepeckiej 26A, 60-465 Poznań

The description of the behaviour of the ultrafine-grained titanium by the constitutive model of elasto-viscoplasticity

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Abstract

The main objective of the present paper is the description of the behaviour of the ultrafine-grained (UFG) titanium by the constitutive model of elasto-viscoplasticity with the development of the identification procedure. We intend to utilize the constitutive model of the thermodynamical theory of elasto-viscoplasticity for description of nanocrystalline metals presented by Perzyna (2010)[1]. The identification procedure is based on experimental observation data obtained by Jia et al. (2001)[4] for ultrafine-grained titanium and by Wang et al. (2007) [5] for nanostructured titanium. Hexagonal close-packed (hcp) ultrafine-grained titanium processed by sever plastic deformation (SPD) has gained wide interest due to its excellent mechanical properties and potential applications as biomedical implants.

Keywords: elasto-viscoplasticity, ultrafine-grained titanium, uniaxial compression

1. The constitutive model

We propose to introduce some simplification of the constitutive model developed by Perzyna (2010)[1] by assuming that the internal state variable vector $\boldsymbol{\mu} = (\in^p, d, \boldsymbol{\xi})$ consists of two scalars and one tensor, i.e. $\in^p$ denotes the equivalent viscoplastic deformation, d defines the mean grain diameter and $\boldsymbol{\xi}$ is the microdamage second order tensor, with the physical interpretation that $(\boldsymbol{\xi} : \boldsymbol{\xi})^{1/2} = \xi$ defines the volume fraction porosity. The equivalent inelastic deformation $\in^p$ describes the dissipation effects generated by viscoplastic flow phenomena, the microdamage tensor $\boldsymbol{\xi}$ takes into account the anisotropic intrinsic microdamage mechanisms on internal dissipation and d describes the dynamic grain growth during intensive deformation process. We postulate the plastic potential function in the form $f = f(J_1, J_2, \vartheta, \boldsymbol{\mu})$, where J_1, J_2 denote the first two invariants of the Kirchhoff stress tensor $\boldsymbol{\tau}$ and ϑ is absolute temperature. The evolution equations are assumed as follows

$$\mathbf{d}^p = \Lambda \mathbf{P}, \quad \mathrm{L}_{\boldsymbol{v}} \boldsymbol{\xi} = \boldsymbol{\Xi}, \quad \dot{d} = D \tag{1}$$

where

$$\Lambda = \frac{1}{T_m} \langle \Phi(\frac{f}{\kappa} - 1) \rangle, \qquad \mathbf{P} = \frac{\partial f}{\partial \boldsymbol{\tau}}\Big|_{\boldsymbol{\xi}=const} \left(\left|\left| \frac{\partial f}{\partial \boldsymbol{\tau}} \right|\right| \right)^{-1}, \tag{2}$$

$\mathbf{d}^p$ denotes the rate of inelastic deformation tensor, T_m denotes the relaxation time for mechanical disturbances, the isotropic work–hardening–softening function $\kappa = \hat{\kappa}(\in^p, \vartheta, \boldsymbol{\xi}, d)$, Φ is the empirical overstress function, the bracket $\langle \cdot \rangle$ defines the ramp function, $\mathrm{L}_{\boldsymbol{v}}$ denotes the Lie derivative and $\boldsymbol{\Xi}$ and D denote the evolution functions which have to be determined.
Let us assume that the intrinsic microdamage process is generated by growth mechanism only. Based on the heuristic suggestions and taking into account the influence of the stress triaxiality and anisotropic effects on the growth mechanism we assume the evolution equation for the microdamage tensor $\boldsymbol{\xi}$ as follows

$$\mathrm{L}_{\boldsymbol{v}} \boldsymbol{\xi} = \frac{\partial g^*}{\partial \boldsymbol{\tau}} \frac{1}{T_m} \langle \Phi[\frac{I_g}{\tau_{eq}(\vartheta, \boldsymbol{\mu})} - 1] \rangle. \tag{3}$$

The tensorial function $\frac{\partial g^*}{\partial \boldsymbol{\tau}}$ represents the mutual micro(nano)crack interaction for growth process, $\tau_{eq} = \hat{\tau}(\vartheta, \boldsymbol{\mu})$ denotes the threshold stress function for growth mechanism, $I_g = b_1 J_1 + b_2 \sqrt{J_2^{'}}$ defines the stress intensity invariant, $J_2^{'}$ denote the second invariant of the Kirchhoff stress deviator tensor, b_i $(i = 1, 2)$ are the material coefficients which can depend on d. In the evolution equation (3) the function $g = \hat{g}(\boldsymbol{\tau}, \vartheta, \boldsymbol{\mu})$ plays the fundamental role, and we introduce the denotation $\frac{\partial g^*}{\partial \boldsymbol{\tau}} = \frac{\partial \hat{g}}{\partial \boldsymbol{\tau}} \left(\left|\left| \frac{\partial \hat{g}}{\partial \boldsymbol{\tau}} \right|\right| \right)^{-1}$. Assuming that the dynamic grain growth is the rate dependent mechanism (cf. Perzyna (2010)[1]) we postulate

$$\dot{d} = \frac{\hat{\mathcal{G}}(\vartheta, \boldsymbol{\mu})}{T_m} \langle \Phi \left[\frac{I_d}{\tau_d(\vartheta, \boldsymbol{\mu})} - 1 \right] \rangle, \tag{4}$$

where $\mathcal{G} = \hat{\mathcal{G}}(\vartheta, \boldsymbol{\mu})$ is the material function, $I_d = c_1 J_1 + c_2 \sqrt{J_2^{'}}$ represents the stress intensity invariant for grain growth, c_i $(i = 1, 2)$ are the material coefficients which may depend on d, and $\tau_d = \hat{\tau}_d(\vartheta, \boldsymbol{\mu})$ denotes the threshold stress for dynamic grain growth mechanism. For previous theoretical and experimental works on this problem please consider following papers, e.g. Chen et al. (2006)[6], Kumar et al. (2003)[7], Meyers et al. (2006)[8] and Nowak and Perzyna (2011) [9].

2. The identification procedure

The identification procedure consists of two parts. In the first part the determination of the material functions and the material constants involved in the description of the dynamic yield criterion Eqn (6) is presented. As an experimental base the results concerning experimental observation for ultrafine-grained titanium obtained by Jia et al. (2001)[4] and for nanostructured titanium obtained from the compression tests at high strain rates ($10^3 - 10^4$ s^{-1}) by Wang et al. (2007) [5]. The second part is focused on the determination of the material functions and the material constants appeared in the evolution equations (3) and (4). However, before our final approach to the identification of all parameters of our model, we assume that the grain size is constant, function $\mathcal{G} = 0$ in Eqn (4). Let us also assume that for simplicity

we use the scalar internal state variable $\xi = (\boldsymbol{\xi} : \boldsymbol{\xi})^{1/2}$ instead of microdamage tensor $\boldsymbol{\xi}$ and we propose the evolution equation for the porosity ξ as follows (cf. Perzyna (2005) [2])

$$\dot{\xi} = \dot{\xi}_{grow} = \frac{g^*(\xi,\vartheta)}{T_m \kappa_0(\vartheta)} \left[I_g - \tau_{eq}(\xi,\vartheta,\in^P) \right] \tag{5}$$

where $T_m \kappa_0(\vartheta)$ denotes the dynamical viscosity of a material and $\tau_{eq}(\xi,\vartheta,\in^P)$ is the void growth threshold stress.

Let us introduce the particular form for the plastic potential function as follows $f = \left[J_2^{'} + n\left(\vartheta, d\right) \left(\boldsymbol{\xi} : \boldsymbol{\xi}\right)^{1/2} \left(J_1^2\right) \right]^{\frac{1}{2}}$, where $J_2^{'}$ denotes the second invariant of the stress deviator of the Kirchhoff stress $\boldsymbol{\tau}$ and $n = n\left(\vartheta, d\right)$ is the material function.
From Eqn $(1)_1$ and Eqns (2) we have the dynamical yield criterion in the form

$$\left[J_2^{'} + n\left(\vartheta, d\right) \left(\boldsymbol{\xi} : \boldsymbol{\xi}\right)^{1/2} \left(J_1^2\right) \right]^{\frac{1}{2}} = \kappa \left[1 + \Phi^{-1} \left(\frac{\sqrt{3}}{2} T_m \dot{\in}^P \right) \right]. \tag{6}$$

where $\kappa = \kappa_0(\vartheta) + \kappa^*(\in^P)$ is the isotropic work-hardening-softening function. Taking advantage of the description of the microshear banding effects for nanocrystalline titanium we can propose the relation for the relaxation time (cf. Perzyna (2010)[1], Pęcherski (1998) [3])

$$T_m = T_m^0 \left[1 - f_{ms}^0 \frac{1}{1 + \exp\left(a - b \in^P\right)} \right] \left(\frac{\dot{\in}^P}{\dot{\in}_s^P} - 1 \right)^{\frac{1}{p}}, \tag{7}$$

where T_m^0, f_{ms}^0, a, b, p and $\dot{\in}_s^P$ are material function of d.

To integrate our set of the nonlinear equations (see Eqn (5), Eqn (6) and Eqn (7)) the return mapping algorithm is used to solve the system of above equations. All operators are performed at the end of time increment. We applied our algorithm within ABAQUS/EXPLICIT code by writing a user-material subroutine. We consider the compression quasistatic and dynamic processes (the initial boundary-value problems) for the cylindrical specimen to investigate the deformation mode and to compare the obtained results with those observed experimentally during the processes of direct impact compression test, cf. Jia et al. (2001) [4] and Wang et al. (2007) [5].

The sample is modeled with 3D solids elements (type C3D8R in the ABAQUS). In numerical simulations the specimen is supported by a transmitting rod and is impacted by a second moving one with an imposed velocity. Both rods in contact with sample are chosen as an elastic bodies with finite friction. Simulation leads to plastic strain and strain rates in the same range as in experimental test of Wang et al. (2007) [5]. The elasto-viscoplasticity model parameters are determined for specimen with different average grain size for the course grained titanium $d = 30\ \mu m$ (CG) and the ultrafine-grained titanium $d = 260\ nm$ (UFG). In each case we have started our computations assuming at the beginning a broad range of feasible parameters. After initializing and after final determination of material constants which minimising the residua of the constitutive model and the experimental data we apply our model in numerical simulation of uniaxial compression and we have obtain the final state of strain and stress.

3. Final comments

There is our hope that proposed identification procedure for the thermodynamical theory of elasto-viscoplasticity of nanocrystalline metals may be used as a base for the description of the behaviour of hexagonal close-packed ultrafine-grained titanium processed by sever plastic deformation and may allow to do the investigation of plastic strain localization and fracture phenomena in nano-mechanical processes, for instance compare: Asaro et al. (2003) [10], Zhu et al. (2005) [11] and Zhu et al. (2003) [12]. These coming results and excellent mechanical properties of this kind of titanium make potential applications possible as biomedical implants.

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