The identification procedure for the constitutive model of elasto–viscoplasticity with microdamage and dynamic grain growth mechanisms describing the behaviour of nanocrystalline iron

Zdzisław Nowak and Piotr Perzyna*
Department of Mechanics of Materials
Institute of Fundamental Technological Research
Polish Academy of Sciences
Pawińskiego 5B, 02–106 Warsaw, Poland
e-mail: znowak@ippt.gov.pl, pperzyna@ippt.gov.pl

Abstract

The main objective of the present paper is the development of identification procedure of the constitutive model of elasto-viscoplasticity describing the behaviour of nanocrystalline iron. We intend to utilize the constitutive model presented by Perzyna (2010). The procedure is based on experimental observation data obtained by Jia, Ramesh and Ma (2003) for consolideted iron with average grain sizes from tens of nanometers to tens of microns under uniaxial compression over a wide range of strain rates and by Wei et al. (2004) for ultrafine-grained iron processed by severe plastic deformations.

Keywords: elasto-viscoplasticity, nanocrystalline iron, uniaxial compression

1. Introduction

The main objective of the present paper is the development of identification procedure of the constitutive model of elasto-viscoplasticity describing the behaviour of nanocrystalline iron. Only *bcc* metals will be covered in this description, because they are the classes of metals for which systematic experimental observation data sets are available. An investigating of the deformation mechanisms is important for understanding, controlling and optimizing the mechanical properties of nanocrystalline metals. Strengthening with grain size refinement in metals and alloys with an average grain size of 100 nm or larger has been well characterized by the Hall-Petch (H-P) relationship, where dislocation pile-up against grain boundaries along with other transgranular dislocations mechanisms are the dominant strength-controlling processes. When the average, and entire range of, grain sizes is reduced to less than 100nm, the dislocation operation becomes increasingly more difficult and grain boundary-mediated processes become increasingly more important. The principal short-range barrier, the Peierls-Nabarro stress, is important for ultrafine crystalline *bcc* metals. Experimental observations have shown that nanosized grains rotate during plastic deformation and can coalesce along directions of shear, creating larger paths for dislocation movement. Many results have shown that nanocrystalline materials exhibit the grain size and strain rate dependent mechanical behaviors, the most recent relative review can be seen in Mayers et al. (2006). To understand this sort of mechanical behaviour, several models have been proposed recently using the concept of a two-phase composite. Zhu et al. (2005) developed a polycrystalline constitutive theory based on the model of Asaro et al. (2003) for deformation mechanisms in nanocrystalline metals and the extended aggregate Taylor model by Asaro and Needleman (1985). Despite the successes provided by these models, the effects of grain size and strain rate (especially in a wide strain rate range) on the mechanical behaviour of nanocrystalline materials are not well described in term of their main deformation mechanisms as yet. The deformation mechanism of the nanocrystalline material is very complicated. Even for a same material, the deformation mechanism will also change with the further deformation. For example, the shear band evolution phenomena during the inelastic deformation process have been observed in the compression tests Jia et al. (2003), this indicates that the deformation will become non-uniform in the deformation proces. In this paper, we will be focused on the mechanical behaviour of the nanocrystalline metals in viscoplastic strain range. The developed model will be used to simulate the grain size and strain rate dependent mechanical behaviour of bcc nanocrystalline materials, and the simulation results for bcc nanocrystalline materials will be compared with Jia et al. (2003) experimental data for pure iron. Finally, further discussion will be presented for the uniaxial stress–strain response, shear localization behaviours and strain rate sensitivity of bcc nanocrystalline metal.

2. The constitutive model

The model is developed within the thermodynamic framework of the rate type covariance constitutive structure with a finite set of the internal state variables, cf. Perzyna (2010). We assume that a set of internal state variables $\boldsymbol{\mu} = (\in^p, \boldsymbol{\xi}, d)$ consists of two scalars and one tensor, namely the equivalent inelastic deformation $\in^p$, the second order microdamage tensor $\boldsymbol{\xi}$ with the physical interpretation that $(\boldsymbol{\xi} : \boldsymbol{\xi})^{1/2} = \xi$ defines the volume fraction porosity and d the mean grain diameter. 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. Let us introduce the plastic potential function $f = f(J_1, J_2, \vartheta, \boldsymbol{\mu})$, where J_1, J_2 denote the first two invariants of the stress tensor $\boldsymbol{\tau}$, ϑ is absolute temperature. We postulate the evolution equations as follows

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

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where $\mathrm{L}_{\boldsymbol{v}}$ denotes the Lie derivative. For elasto–viscoplastic model of a material we assume

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

T_m denotes the relaxation time for mechanical disturbances. To describe the microshear banding effects let us assume that the relaxation time T_m depends on the active microshear bands fraction β_{ms}, on the rate of equivalent viscoplastic deformation $\dot{\in}^p$ and the grain diameter d, i.e. $T_m = T_m(\beta_{ms}, \dot{\in}^p, d)$. Additionally we introduce the simplification as follows $T_m = T_m^0(d)\phi_1(\beta_{ms}, d)\phi_2(\dot{\in}^p, d)$. 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, $\boldsymbol{\Xi}$ and D denote the evolution functions which have to be determined.

3. The determination of the evolution functions

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

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

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, 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)) we postulate

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

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. The evolution equations (3) and (4) determine the evolution functions $\boldsymbol{\Xi}$ and D, respectively.

4. The identification procedure

Let us introduce the particular form for the plastic potential function as follows

$$f = \left[J_2' + n\,(\vartheta, d)\,(\boldsymbol{\xi} : \boldsymbol{\xi})^{1/2}\left(J_1^2\right)\right]^{\frac{1}{2}}, \quad (5)$$

where J_2' denotes the second invariant of the stress deviator of the Kirchhoff stress $\boldsymbol{\tau}$ and $n = n\,(\vartheta, d)$ is the material function. From $(1)_1$, $(2)_1$ and (5)we have the dynamical yield criterion in the form

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

Taking advantage of the description of the microshear banding effects for nanocrystalline iron proposed by Perzyna (2010) we have the relation for the relaxation time

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

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

We propose that 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 (6) is presented. As an experimental base the results concerning a set of stress-strain responses of the consolidated iron obtained from the quasistatic compression tests and at high strain rates ($3\mathrm{x}10^3 - 6\mathrm{x}10^3$ s^{-1}) for several grain sizes by Jia, Ramesh and Ma (2003) are assumed. The second part is focused on the determination of the material functions and the material constants appeared in the evolution equations (3) and (4). To do that we consider the compression quasistatic and dynamic processes (the initial boundary-value problems) for the prismatic specimen to investigate the deformation mode and to compare the obtained results with those observed experimentally during the processes of shear banding, cf. Jia, Ramesh and Ma (2003). We used also the experimental investigations of the development of adiabatic shear banding in ultrafine grained iron processed by sever plastic deformation performed by Wei et al. (2004) to make the similar identification analysis.

References

[1] Asaro R.J., Krysl P., Kad B., Deformation mechanism transitions in nanoscale fcc metals, *Philosophical Magazine Letters*, **83**, pp. 733–743, 2003.

[2] Asaro R.J., Needelman A., Overview no. 42. Texture development and strain hardening in rate dependent polycrystals, *Acta Metallurgica*, **33** (6), pp. 923–953, 1985.

[3] Jia D., Ramesh K.T., Ma E., Effects of nanocrystalline and ultrafine grain sizes on constitutive behaviour and shear bands in iron, *Acta Materialia*, **51**, 3495-3509, 2003.

[4] Meyers M.A., Mishra A., Benson D.J., Mechanical properties of nanocrystalline materials, *Progress in Materials Science*, **51**, 427–556, 2006.

[5] Nowak Z., Perzyna P., The identification procedure for the constitutive model of elasto–viscoplasticity with microdamage and dynamic grain growth mechanisms describing the behaviour of nanocrystalline iron during quasistatic and dynamic loading processes, *Proc. of Conf. on Modelling of Continuous Media with Microstructure*, Łódź, 2011.

[6] Perzyna P., The thermodynamical theory of elasto-viscoplasticity for description of nanocrystalline metals, *Engineering Transactions*, **58** (1-2), 15-74, 2010.

[7] Wei Q., Kecskes L., Jiao T., Hartwig T., Ramesh K.T., Ma E., Adiabatic shear banding in ultrafine-grained Fe processed by severe plastic deformation, *Acta Materialia*, **52**, 1859–1869, 2004.

[8] Zhu B., Asaro R. , Krysl P., Bailey R., Transition of deformation mechanisms and its connection to grain size distribution in nanocrystalline metals, *Acta Mater.*, **53**, pp. 4825-4838, 2005.