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Dislocation based multilevel model for elastic-plastic deformation of polycrystalline materials

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Abstract. The main aim of the work is to study the Portevin–Le Chatelier effect. The occurrence of the effect is closely connected to the phenomenon of dynamic strain ageing, i.e. the additional pinning of mobile dislocations by foreign atoms diffusing into the dislocation core during their arrest at obstacles, e.g. forest dislocation. The description of interaction of dislocation with impurities plays a great role, that`s why it is necessary to develop a several submodels: dislocation submodel for the interaction between dislocations and dislocation submodel for the interaction between dislocations and impurities. The multilevel approach based on using the internal variables, i.e. parameters describing the evolution of meso- and microstructure of the material, was applied to construct the model. The approach to model the dislocation structure is based on introduction of homogeneous dislocations densities on each slip system and obtaining evolutionary equations describing the mechanisms of their generation and interaction. The deformation mechanisms are evaluated and evolution of structural parameters during the process of deformation is analyzed. The dislocation submodel for the interaction between dislocations and impurities will be described in the next papers.

1. Introduction

The Portevin–Le Chatelier (PLC) effect manifests itself as an unstable plastic flow on the macrolevel. It is observed in a wide class of plastic materials under certain regimes of strain rate and temperature. The PLC effect is mostly studied through tensile testing either at constantly applied stress rate (‘soft’ loading) or at constantly applied strain rate (‘hard’ loading). The typical shapes of the stress–strain curves displayed in those two cases are, respectively, of staircase type, with bursts of plastic strain at almost constant stress, and serrated, with sudden stress drops at almost constant strain.

One of the main problems we have in the process of plastic deformation is establishing a necessary condition for loss of material stability and establishing the boundaries of the PLC effect range. A huge number of publications is devoted at the present time [1, 2] to studying of the general regularities and the character of the distribution of inhomogeneous plastic deformation at meso- and macro-scales, because the serrated yielding is detrimental and leads to loss of formability and ductility.

Numerous experiments of discontinuous plasticity have demonstrated that the plastic behavior of materials under constant loading depends on inhomogeneities properties of the material and the cooperative motion of large number of dislocations at different scale levels, from nano- to macroscale. Experimental studies of the internal structure evolution, dislocation substructures and point defects, which influence physical and mechanical processes of the materials, are very difficult and expensive. Therefore, in the last decades, there is an increasingly more need for constructing mathematical models of different scale levels.

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The main mechanism responsible for the manifestation of the PLC effect is dynamic strain aging (DSA), it results from the interaction between solute atoms and mobile dislocation, whereas the mobile dislocation is temporarily arrested in the slip path by obstacles, e.g. forest dislocation, solute atom aggregations, etc.

The majority of researchers (A. Benallal, A. Bertram, T. Böhlke, L.P. Kubin, Y. Estrin, R. Larsson, S.-Y. Yang, D. Yu, X. Chen, S. Zhang and others) use macro phenomenological models of inelastic deformation to describe the effects associated with dynamic strain aging (DSA) [1]. The original formulation of the phenomenological viscoplastic model of strain aging proposed by Kubin and Estrin (1985) is based on an implicit mathematical description of homogeneous material exhibiting negative strain rate sensitivity [3]. Macro phenomenological models based on the macroscopic description of the deformation establish the relationships between the parameters at the macrolevel, but they don't consider the microstructure of the material.

The crystal plasticity based models (J. Alcala, H. Askari, R.A. Austin, D.L. McDowell, J. Balik, P. Lukac, M.S. Bharathi and others) allow to simultaneously analyze deformation processes at the macrolevel and to describe explicitly inelastic deformation mechanisms, material internal structure and its evolution at lower scale levels. A brief review of models, which are based on crystal plasticity, devoted to the description of the materials deformation, associated with the diffusion processes, in wide ranges of strain rates and temperatures is given in [2]. One of the important issues that arise in construction of this class of models: 'closing' set of relationships, a large number of parameters and their identification, is the problem of numerical implementation.

The article discusses physical mechanisms of serrated yielding. Plastic deformation is associated with a non-uniform motion of elementary carriers of plastic flow, i.e. dislocations (in time and space). Thus, for a correct description of plastic deformation, its heterogeneity and taking into account all its attendant real physical mechanisms, there is need to study the material behavior not only on the macrolevel, but on a lower meso- and microstructural levels, that is why a number of scientists attempted to construct dislocation dynamics models (A. Alankar, A. Arsenlis, K.M.Davoudi, L. Kiely, D. Li, H. Zbib, C. Reuber, M. Zecevic, M. Knezevic, M. Lebedkin and others).

This paper considers the multilevel mathematical model [4] based on the crystal plasticity theories, proposed to describe the Portevin–Le Chatelier effect. The description of interaction of dislocation with impurities plays a great role. The approach to model the dislocation structure is based on introduction of homogeneous dislocations densities on each slip system and obtaining evolutionary equations describing the mechanisms of their generation and interaction. The dislocation submodel for describing the mechanisms of the interaction between dislocations and impurities is in development stage and it isn`t considered in the present paper.

2. PLC constitutive model

Using the two-level models for describing the PLC effect isn't correct, because it is impossible to take into account the changes of the internal stresses of the material (the critical shear stress on slip systems) in the process of inelastic deformation caused by dynamic strain aging in the frame of two-level models. To describe the phenomenon of the Portevin–Le Chatelier effect we produced three-level model based on the crystal plasticity theories by applying dislocation submodel.

The generic structure of direct three-level model has been presented in [5]. In this model, the hierarchy of scale levels is defined as follows: macrolevel (representative volume of polycrystalline material) – mesolevel-1 (the level of the crystallite (grain, subgrain)), mesolevel-2 (grain, subgrain, fragment). Mesolevel-1 is used to describe the processes of hardening and of plastic deformation in terms of shear on the slip systems of a crystallite. Mesolevel-2 is applied to describe complex behaviour of the defect structure evolution and the evolution of dislocations densities. The general problem is facilitated by the definition of three subtasks: 1) determining the stress-strain state, 2) determining of the temperature, and 3) the diffusion. These subtasks can be realize using a dislocation submodel.

The system of relation of material constitutive model with internal variables at the macrolevel includes a set of three groups of equations (state (constitutive relations), evolutionary and closing):

$$\mathbf{\Sigma}^r = \mathbf{F}_r(\mathbf{P}_\alpha, \mathbf{J}^e_\gamma); \quad \mathbf{J}^{ir}_\delta = \mathbf{R}_{r\delta}(\mathbf{P}_\alpha, \mathbf{J}^i_\beta); \quad \mathbf{J}^{er}_\gamma = \mathbf{C}_{r\gamma}(\mathbf{P}_\alpha, \mathbf{J}^i_\delta), \tag{1}$$

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where $\boldsymbol{\Sigma}, \boldsymbol{\Sigma}^r$ is a measure of the stress and its objective rate of change; $\mathbf{F}_r$, $\mathbf{R}_{r\delta}$, $\mathbf{C}_{r\gamma}$ are tensor functions or simple (for example, differential) operators over tensor-valued arguments; $\mathbf{P}_\alpha$ - parameters of thermomechanical and non-thermomechanical nature; the superscript «*r*» represents a derivative, that does not depend on the coordinate system choice; $\mathbf{J}_\gamma^e$ are the explicit internal variables which enter the structure of the constitutive relations; $\mathbf{J}_\beta^i$ are the implicit internal variables, characterizing structure evolution and related to deeper scale levels [6].

Strain rate tensor is additively decomposed into elastic and plastic parts, the tensor is applied at the macrolevel and mesolevel-1. The strain rates calculation at nodes is performed using finite element method (FEM), the description of the evolution of dislocations densities, barriers and shear strain rate on the *k*-th slip system are considered at the mesolevel-2. Asymmetric measure of the deformed state and the modified Hooke's law are used at all levels [7].

The main mode of plastic deformation is the slip of edge dislocations. At the mesolevel-1, the response (stress) of the crystallite is determined from the velocity gradient, which is transmitted from the macrolevel. The velocities of dislocation movement on the slip system are transmitted from the mesolevel-2 to the mesolevel-1, the inelastic part of the velocity gradient and the components of the Cauchy stress tensor are established using Hooke's law and compute using the FEM.

3. Dislocation model (mesolevel-2)

The dislocations velocity may decrease due to their interaction with each other and with other defects in nonideal crystals. Dislocation motion can be hindered by dislocation interaction. The description of dislocation evolution takes into account the basic mechanisms: generation of dislocations by Frank-Read sources, annihilation of dislocations, and the formation of dislocation barriers (immobilization), detaching barriers by thermally activated mechanism or the respective critical shear stress (mobilization). The total dislocation density can be decomposed additively into the densities of mobile and immobile dislocations: $\rho_m^{(k)} = \rho_m^{(k)} + \rho_m^{(k)}$. It is proposed that, during the motion glide edge dislocations annihilate mutually with dislocations of opposite sign, the mobile and immobile dislocation densities can be divided into positive and negative parts depending on the location of the extra plane:

$$\begin{aligned} \rho_m^{(k)} &= \rho_{m+}^{(k)} + \rho_{m-}^{(k)}, \\ \rho_{im}^{(k)} &= \rho_{im+}^{(k)} + \rho_{im-}^{(k)}. \end{aligned} \quad (2)$$

In the reference configuration, the initial densities of positive and negative dislocations are supposed to be equal: $\rho_{m+}^{(k)}|_{t=0} = \rho_{m-}^{(k)}|_{t=0} = \dfrac{\rho_{m0}^{(k)}}{2}|_{t=0}$.

The positive (negative) mobile dislocations velocity depends on the temperature of the material under loading, actual and critical resolved shear stress on the slip system and is defined as follows [8]:

$$v_{m\pm}^{(k)} = v_0^{(k)} \exp\left(-\Delta G (\kappa\theta)^{-1} \left(1 - \left(\left|\tau^{(k)}\right| \left(\tau_{\text{crit}}^{(k)}\right)^{-1} \right)^p \right)^q \right), \quad (3)$$

where ΔG is the activation energy of dislocation movement, κ is Boltzmann constant, $\tau^{(k)}, \tau_c^{(k)}$ are the resolved shear stress and critical resolved shear stress, θ is the absolute temperature, *p*, *q* are dimensionless parameters. The critical resolved shear stress for positive and the negative dislocations in first-order match together.

The critical resolved shear stress depends on the total dislocation density and dislocation interactions on different slip systems:

$$\dot{\tau}_{\text{crit}}^{(i)} = |\mathbf{b}| \sum_{j=1,24} C_{ij} \left(\rho_m^{(i)} + \rho_{im}^{(i)} \right)^{1/2}, \quad (4)$$

where C_{ij} is the dislocation interaction matrix, $\mathbf{b}$ is the Burgers vector.

The equations describing the evolution of mobile and immobile dislocation densities are presented in the following way:

$$\begin{aligned} &\rho_m^{(k)} = \rho_{m+}^{(k)} + \rho_{m-}^{(k)}, \\ &\rho_{im}^{(k)} = \rho_{im+}^{(k)} + \rho_{im-}^{(k)}. \\ &\dot{\rho}_{m\pm}^{(k)} = \dot{\rho}_{gen\pm}^{(k)} + \dot{\rho}_{mob\pm}^{(k)} - \dot{\rho}_{imm\pm}^{(k)} - \dot{\rho}_{ann\,m\pm}^{(k)} - \dot{\rho}_{ann(m\pm im\mp)}^{(k)}, \\ &\dot{\rho}_{im\pm}^{(k)} = \dot{\rho}_{imm\pm}^{(k)} - \dot{\rho}_{mob\pm}^{(k)} - \dot{\rho}_{ann(m\mp im\pm)}^{(k)}. \end{aligned} \tag{5}$$

Here, the subscripts *gen*, *ann*, *imm* and *mob* refer to the generation dislocations, annihilation, trapping (locking by the obstacles: grain boundaries, forest dislocations, second-phase inclusions) and mobilization of dislocations, respectively.

In equation (5) the change rate of mobile dislocations density, both positive and negative, consists of 5 terms: dislocations generation rate in the grain by Frank-Read sources $\dot{\rho}_{gen\pm}^{(k)}$; an increase of the mobile dislocations density by detachment dislocations from barriers $\dot{\rho}_{mob\pm}^{(k)}$; a decrease of the mobile dislocations density by locking the obstacles (of dislocation origin or non-dislocation origin)on the slip systems $\dot{\rho}_{imm\pm}^{(k)}$; a decrease of the mobile dislocations density at dislocations annihilation of opposite signs $\dot{\rho}_{ann\,m\pm}^{(k)}$; a decrease of the mobile dislocations density at the annihilation of mobile and immobile dislocations of opposite signs $\dot{\rho}_{ann(m\pm im\mp)}^{(k)}$. An increase of the immobile dislocations density occurs due to inverse processes.

The generation rate depends on the density of active sources of dislocations and may be written as follows from [9]:

$$\dot{\rho}_{nuc}^{(k)} = \rho_s^{(k)} \frac{v^{(k)}}{h_{ann}}, \tag{6}$$

where $\rho_s^{(k)}$ is the density of active sources of dislocations; $h_{ann} \square (\rho_m)^{-1/2}$ is the distance between newly formed dislocations, when the dislocations of opposite signs approach each other in a smaller distance, they annihilate.

During the process of plastic deformation, the dislocation density increases, and the number of active sources increases too. The authors [10] assume that the density of active sources is proportional to the density of dislocations. Then the generation rate of dislocations is taken in the following way:

$$\dot{\rho}_{gen}^{(k)} = \rho_s^{(k)} \frac{v^{(k)}}{h_{ann}} = v^{(k)} \left(\rho_m\right)^{3/2}. \tag{7}$$

During the motion, dislocations will tend to interact. When they are in the same plane on a critical distance h_{ann} ,they repel each other if they have the same sign, and they annihilate reciprocally if they have opposite signs (producing a perfect crystal). The rate of dislocation annihilation is taken in the following way [8]:

$$\begin{aligned} &\dot{\rho}_{ann\,m+}^{(k)} = \dot{\rho}_{ann\,m-}^{(k)} = h_{ann} \rho_{m+}^{(k)} \rho_{m-}^{(k)} (v_{m+}^{(k)} + v_{m-}^{(k)}), \\ &\dot{\rho}_{ann(m\pm im\mp)}^{(k)} = h_{ann} \rho_{im\pm}^{(k)} \rho_{m\mp}^{(k)} v_{m\mp}^{(k)}. \end{aligned} \tag{8}$$

The critical shear stress is determined by the current state of the defect densities on the slip system. The average dislocations velocities are determined by the shear stress, temperature, and defects density. The average dislocations velocities determined at the mesolevel-2 are used on the mesolevel-1, where shear strain rate is set according to the Orovan's equation.

4. Results

Numerical experiments have been carried out to determine the change in the density of dislocations, changes in critical stresses on slip systems over time under uniaxial loadings along the [100] direction.

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Under such loading there are eight equal active slip systems, critical stresses on these slip systems changes in the same way.

Figure 1 shows the dependence diagram of critical shear stress – inelastic strain with under a constant number of dislocation sources and in the case when the sources density increases.

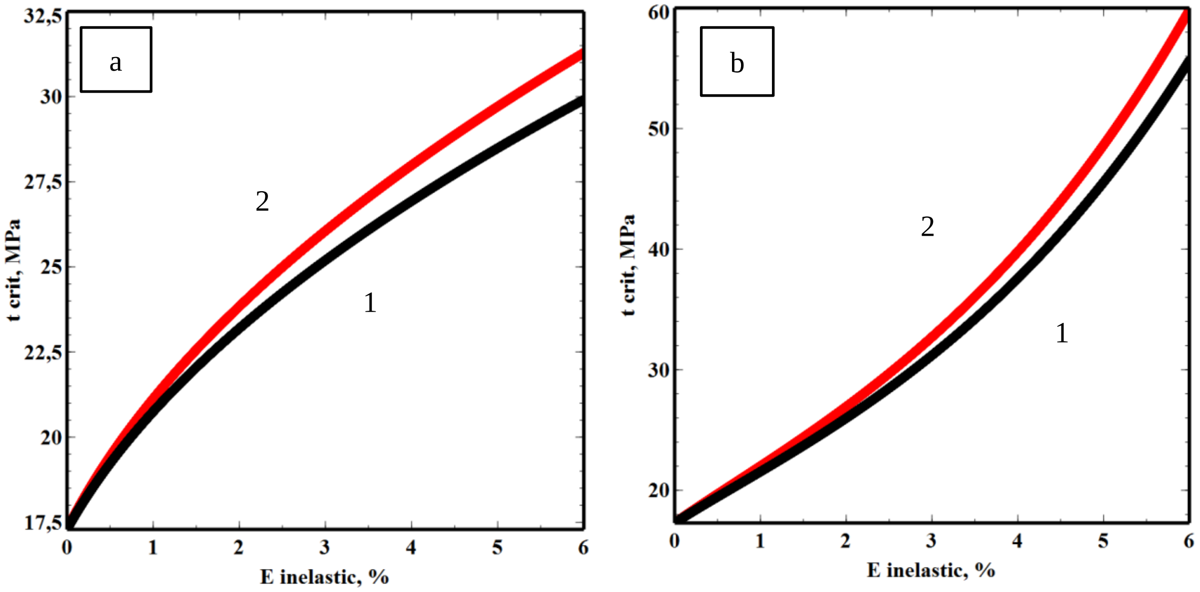

Figure 1. The critical shear stress – inelastic strain on active (1) and inactive (2) slip system with: a) constant number of dislocation sources, b) the increase of sources density.

Figure 2 shows the dependence diagram of critical shear stress – mobile dislocations density under a constant number of dislocation sources and in the case when the sources density increases.

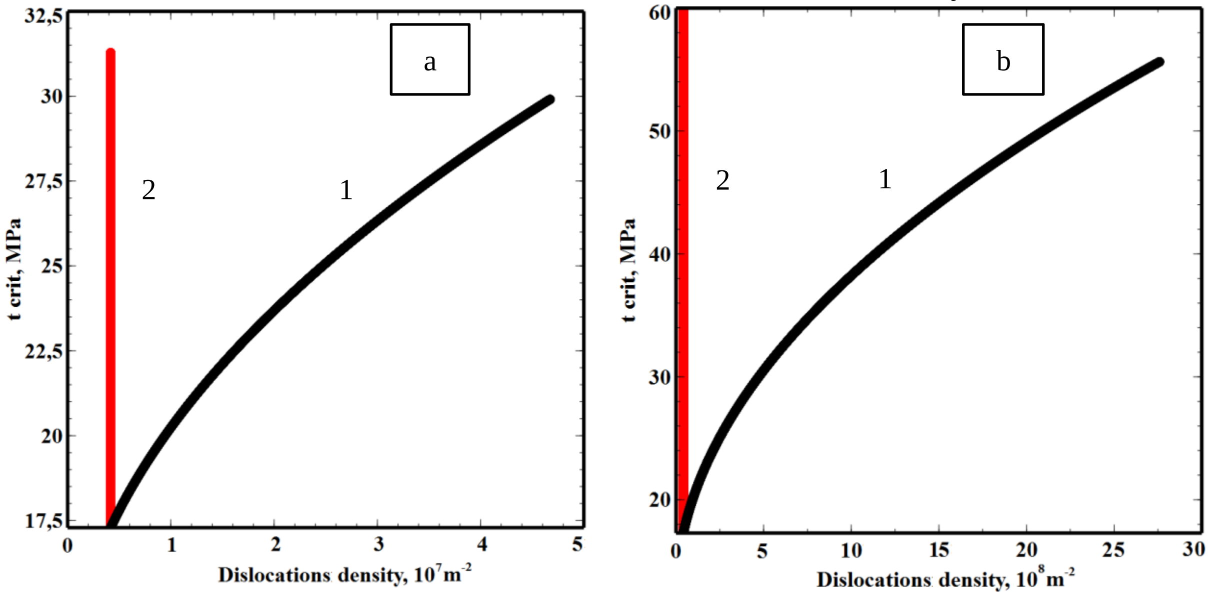

Figure 2. The critical shear stress – mobile dislocations density on active (1) and inactive (2) slip system with: a) constant number of dislocation sources, b) the increase of sources density.

5. Conclusion

In this paper, we consider multilevel constitutive model to describe the serrated yielding, taking into account the dislocation submodel. Only two first terms in the evolution equations for the dislocation

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densities are considered. The numerical experiments have been carried out to determine the change rate of mobile dislocations density and the critical shear stress on slip system over time. The dependence diagrams of critical shear stress – mobile dislocations density, critical shear stress – inelastic strain on active and inactive slip system under uniaxial loadings are obtained. The results of numerical experiments of the developed model graphically demonstrated some features of the deformation behaviour and the evolution of the dislocation structure.

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