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Non-equilibrium approach to prediction of microstructure evolution for metals undergoing severe plastic deformation

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ABSTRACT

Available models of dynamic recrystallization have a number of disadvantages that in most cases make them inapplicable for practical predictions of material microstructure evolution. Both the microstructural and the empirically based approaches do not reflect physical processes leading to evolution of material defect structure in the process of plastic deformation. This work presents an attempt to develop a consistent physically-based model of dynamic recrystallization. This model, accounting for physical nature of processes of material defect structure evolution, should provide a possibility to predict evolution of several different experimentally measurable parameters of material microstructure without introduction of big number of fitting parameters. It is suggested that such a model should be based on equation for evolution of fraction of high-angle grain boundaries (HAGBs) in the process of deformation. It is shown, that the new model gives a possibility to predict the evolution of dislocation cells and grain boundaries in copper-based alloys providing good coincidence with experimental observations. Full 3-dimensional numerical simulation of multidirectional forging of copper is performed utilizing the developed dynamic recrystallization model. The same 3D simulations demonstrate new noteworthy effects connected to inhomogeneous distribution of plastic strain within the bulk of the material and material strain hardening.

1. Introduction

Experimental investigations of severe plastic deformation (SPD) of different metals [1–10] show that changes obtained by different elements of material macrostructure in the process of deformation are non-monotonous and are dependent on the whole set of external factors. Among the most significant properties of microstructure modified in the process of deformation one can distinguish scalar density of dislocations inside cells and in the cell walls [1,2,4,5], average size of dislocation cells, average grain size, dispersion of grain size distribution, aspect ratio (geometrical property characterizing grain shape) of individual grains [1,2] and fraction of high angle grain boundaries (HAGBs) with misorientation angles exceeding 15° [1,2]. Some of these parameters, such as scalar density of mobile/immobile dislocations [8], average grain size and fraction of HAGBs are dynamically interconnected.

All of these parameters can be registered by a precise appraisal of microstructure, obtained by the processed metallic sample after each pass of multidirectional forging (MDF) [1,2], accumulative roll bonding (ARB) [1,3,6], high pressure torsion (HPT) [3,6,11,12] or equal-channel angular pressing (ECAP) [3,6,12], being the most common SPD-processes. A significant number of known works is devoted to investigation of the influence of parameters of microstructure on microhardness, yield stress, strength, ultimate fracture strain and other mechanical parameters of metallic materials [1,3,7,9,12,13]. It is notable that when analysing mechanical properties of the processed materials it can be observed that different SPD processes often result in very similar changes of mechanical properties for the same accumulated strain, differing only in details [1,14]. Nevertheless, these details can be essential for other material properties, such as conductivity [3,9,15], stability of the received microstructure and diffusive properties [3]. Besides, different SPD methods result in a different degree of spatial inhomogeneity of the resulting microstructure. The simplest and hence the most convenient for analysis are SPD processes of multidirectional forging (MDF) and accumulative roll bonding, implementing essentially the same modes of shear deformation. In [1,2] A. Belyakov et al. analysed dynamic recrystallization in copper and steels subjected to a different number of MDF passes. For precise analysis of the dislocation structure appearing in the material, both the X-ray diffraction (XRD) and the electron backscatter diffraction (EBSD) methods [16] were used. Such an analysis provides a possibility to give an adequate

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estimation of scalar density of dislocations in the centre of a dislocation cell/grain (in the present work these dislocations will be referred to as mobile dislocations) as well as in boundaries (these dislocations will be referred to as immobile (or locked) dislocations). In some works (ex. [1]) an average size of a dislocation cell and an average size of a grain are measured independently. In these works, the received size of dislocation cell is always less as compared to the average size of a grain. Having a number of different measurable parameters of material microstructure evolving in the process of deformation, it is natural to raise a question about the role of each individual parameter for the dynamic recrystallization of material. The scheme presented in [17] makes it possible to describe all the main stages of dynamic recrystallization, but the mechanism of transformation of low angle boundaries of subgrains into high angle boundaries of grains remains unclear. A significant role of existing stress concentrators for this process is evident.

On the other hand, from mechanical point of view, two main issues arise in connection with SPD technologies: (i) a possibility to control all the above mentioned microstructural parameters by the process of plastic deformation and (ii) the degree of influence of each of the parameters on the resulting mechanical properties of the material. To date, the latter question is studied to a much better extent [3,9,13]. In order to understand microstructural processes, discover possibilities to control these processes and grasp the limitations imposed by these processes on maximum achievable material properties there is a need for development of new physical models of plastic deformation. These models should explicitly incorporate the above-mentioned parameters of microstructure as model variables. Plasticity models available to date [18,19] are not able to reflect neither the diversity of elements of microstructure evolving in the process of deformation nor the dynamical nature of different transient processes provided by varied process rates. In recent publications [20,21] the authors present 3D FEM simulation of SPD utilizing interesting rheological models. In [21] the authors observe an interesting regime of strain localization by formation of shear bands during ECAP. The most prominent models of dislocation plasticity widely used for simulation of different SPD processes [23–26] were proposed by Y. Estrin et al. [5]. A very peculiar modification of the model [5,6] has been recently proposed in [22]. The modification makes the model more accurate, taking into account strain rate dependence and correcting several imperfections in the initial system of equation. In a number of works the authors simulate evolution of dislocation density in a whole volume of a sample subjected to ECAP process (ex. [23]). Within the framework of these models, it is possible to receive realistic estimations of distributions of dislocation densities within the material as well as estimations of average grain size. Simulations utilizing these models provide significantly more information as compared to purely mechanical simulations using von Mises type limiting condition as a plasticity model [27–29]. Among disadvantages of the approaches originating from [5], one can mention a big number of fitting parameters that do not have a clear physical interpretation and no robust method of experimental evaluation. Another deficiency is a disability to predict evolution of the rest of the above-mentioned parameters of material microstructure.

Based on the approach presented in [30], the paper presents an attempt to establish consistent relationships between different processes associated with evolution of microstructure in metals subjected to SPD. It is particularly noteworthy that simulations utilizing the presented approach provide a possibility to predict scalar density of mobile and immobile dislocations, average size of dislocation cells, average grain size, grain aspect ratio, grain sizes, HAGBs fraction as well as the distribution of these parameters within the bulk of the processed material. The same model gives a possibility to account for the effect of strain hardening on the process of deformation.

2. Models Predicting the Evolution of Material Defect Substructure in the Process of SPD

2.1. Models of Dislocation Plasticity

Within the framework of classical model scalar dislocation density as a function of strain ε is given by [31,32]:ρ_D

$$\rho_D'(\varepsilon) = C + A\cdot\sqrt{\rho_D(\varepsilon)} - B\cdot\rho_D(\varepsilon), \tag{1}$$

where the first two terms $C\sim\delta_0\sigma_y{}^0/Gb^2$ and $A\sim\delta_f/b$ are responsible for dislocation density increase as a result of nucleation on dislocation forest and inclusions and the last term $B = k_\alpha$ stands for annihilation of dislocation pairs. Here G is the material shear modulus, b is the Burgers vector, $\sigma_y{}^0$ is the yielding limiting stress for dislocation free annealed material. Model parameters, δ_f and $k_\alpha$are, in essence, fitting parameters that should be evaluated empirically. For the case of $C = 0$ the equation is transformed into one of the variations of the classical "logistic" differential equation predicting the increase of population with the following saturation to limiting density given by: $\rho_D{}^{\max} = (\delta_f/k_\alpha d)^2$. A solution of the logistic equation has an exponential form with respect to deformation:

$$\rho_D = \rho_D^{\max}\left(1 + \left(\sqrt{\frac{\rho_D^{\max}}{\rho_D^0}} - 1\right)Exp[-B^2\varepsilon/A]\right)^2, \tag{2}$$

where $\rho_D{}^0$ is the initial dislocation density in the deformed material. In this case Eq. (1) can be rewritten as:

$$\frac{d\rho_D}{d\varepsilon} = \frac{\delta_0}{Gb^2}\sigma_y^0 + k_a\rho_D\left(\sqrt{\frac{\rho_D^{\max}}{\rho_D}}\right). \tag{3}$$

Obviously, the model can easily be enriched with additional sources and sinks of dislocations. For example, one can account for annihilation of dislocations at grain boundaries of fine-grained material [25,33]. The central problem here is connected to the evaluation of coefficients for this equation and their dependency on temperature and other state variables. For averaged description of processes within the dislocation subsystem, an energy-based approach can be used. In [32] it is considered that parameters for model Eq. (1) can be presented as $\delta_f = \alpha\eta Gb^3/\varepsilon_L$, $\delta_0 = \delta_f\alpha^{-1}$, where $\alpha\sim0.5$ is the Taylor constant [31,34], $\varepsilon_L = 8eV/b$ is the elastic energy of dislocation unit length [33,34], $\eta\sim0.1$ is the fraction of work of plastic deformation stored in the form of defects [32]. For small strains, by various estimates [35,36] this value should be around 10%. For higher strains the value of η is reduced by several times [36]. Using these parameters, it is possible to receive estimations for logistic equation type kinetic model parameters [32] $\delta_f\sim0.01$ and $\delta_0\sim0.02$. These values are normally utilized for simulations employing the classical model [31]. Dependencies of dislocation annihilation coefficients on temperature T and other state variables were received in a number of papers. Here one can mention the works of Galindo-Nava [37], where the annihilation coefficient is presented as:

$$k_\alpha = \left(\frac{G(T)}{G_0(T)}\right)^2\frac{1}{100b\alpha}. \tag{4}$$

Other equations for k_α were received by A. Vinogradov [38] and G.A. Malygin [31]. The definite form for (4) is given by $G(T)$, that, for different approximations, can have linear (or quadratic for k_α) dependency on temperature, as discussed in [39]. In [37] $G(T)$ is given as an exponential function of temperature:

$$G(T) = (4.74\cdot10^4)Exp[-3.97\cdot10^4T]. \tag{5}$$

In [37] k_α is approximated by:

$$k_\alpha = \frac{2+2\alpha}{1+2\alpha}\frac{b\nu_0}{\overline{V}_D}Exp\left[-\frac{\Delta G}{k_b T}\right], \tag{6}$$