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A study on the texture evolution mechanism of nickel single crystal deformed by high pressure torsion

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ABSTRACT

High pressure torsion (HPT) is one of the most promising severe plastic deformation (SPD) techniques to produce ultrafine-grained (UFG) or nano-grained (NG) materials via introducing very large plastic strain. This study aims to understand the texture evolution mechanism during HPT by examining the nickel single crystal. The predicted textures after different HPT rotation angles based on a three-dimensional crystal plasticity finite element method (CPFEM) model agree well with the experimental measurements. Both the modelling and experiment show that the crystallographic orientation rotates gradually towards different ideal torsion texture components during HPT deformation, and three steady-state stages and two transition stages can be divided according to the texture evolution history. The crystal rotation during HPT process has been partitioned into three components around the radial direction, tangential direction, and axial direction, respectively. The texture evolution history and mechanism have been examined and discussed in details.

1. Instruction

In recent years, severe plastic deformation (SPD) has been the subject of intensive interest owing to the exceptional ability of producing ultrafine-grained (UFG) or even nanocrystalline structure materials [1–4]. High pressure torsion (HPT) is one of the most promising SPD techniques as the extremely high shear stain can be continuously achieved via simple means [2]. The HPT technique typically has been used to produce UFG materials with unique microstructures and novel mechanical properties from pieces of metals and alloys [4,5].

It has been known that the major deformation behaviours such as grain refinement and work hardening are strongly related to crystallographic texture [6–8]. Currently, texture evolution during the HPT process has been experimentally studied over a wide range of pure metals and alloys, such as aluminium [9,10], nickel [11–13], copper [14,15], and titanium [16]. It was found that the texture formed during HPT could be defined directly from those revealed for the case of torsion texture, but there were significant variations both in the intensity and the relative proportion of each individual ideal component at different stages of HPT straining. Therefore, different ideal components dominated the developed texture at various strain levels of HPT. After processing to the sufficiently large strain level, the typical torsion texture could usually be developed.

The computational modelling can be a powerful tool to understand the texture evolution mechanisms during plastic deformation [17]. Up to now, a great deal of interest has been devoted to simulate the HPT process. The majority of simulation works used the classic finite element method (FEM) which assumes the adopted materials to behave as isotropic work-hardening solids [18–22]. These conventional FEM simulations are capable of presenting some macroscopical plastic deformation characteristics of HPT, such as the distribution of temperature, the evolution of stress and strain, and the change of geometry after deformation. However, they are unable to predict the texture evolution and have little effect in exploring the underlying deformation mechanism at the micro-scale. Analytical or numerical studies of the HPT process, especially using models integrated with crystal plasticity theory, are relatively rare. Estrin et al. [23] proposed an analytical model by combining the dislocation density based constitutive formulation with a particular gradient plasticity frame to describe the deformation behaviour of copper in HPT. Lee et al. [24,25] made further development based on Estrin's model [23] by embedding the dislocation density based constitutive model into a finite element code to simulate the HPT process. The aforementioned investigations focused on the prediction of cell/grain size evolution with the accumulation of dislocation density and did not study the texture evolution

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process. Kratochvil and his co-workers [26,27] established another type of analytical model for the HPT process. The proposed crystal plasticity model was a simplified version based on an assumption of uniform deformation of plane-strain double slip and the texture evolution was not studied neither. Hafok and Pippan [11] constructed a fully-constrained Taylor model which assumes an equality between the local and the macroscopic strain rates to simulate the texture evolution of nickel single crystal during the HPT process. However, owning to the well-known shortcomings of Taylor model as described in [28,29], they did not give satisfactory texture predictions. Besides, in a recent work published by Muszka et al. [30], they have successfully combined the crystal plasticity modelling and three-dimensional digital materials representation approach for the simulation of cyclic torsion (CT) deformation. According to their results, strain inhomogeneities and texture were accurately obtained in the CT process.

In the present study, a three-dimensional crystal plasticity FEM (CPFEM) model, which incorporates crystal plasticity constitutive equations into the finite element framework, has been developed to simulate the texture evolution during the HPT process. The constitutive law in CPFEM is based on the fact that plastic deformation occurs by crystallographic slips on the slip systems and the rotations of the crystal lattices. With the initial distribution of the crystallographic orientation, CPFEM can simulate the change of the orientation for each node and simultaneously calculate hardening and deformation response based on the applied boundary conditions. CPFEM models have been recognized as the best models for the simulation of plastic deformation of crystalline materials and for the prediction of deformation textures [31]. The single crystal was chosen because it eliminates the effect of grain boundary and grain-grain interaction. The simulation results have been compared with the experimental measurements and the texture evolution mechanism in HPT was discussed in details.

2. CPFEM simulation model

2.1. Crystal plasticity theory

Details with regard to the kinematical theory and constitutive relations used in this study can be found in Refs. [32,33].

To overcome the long standing problem of non-uniqueness in the choice of the active slip systems which are inherent in conventional rate-independent theory, the rate-dependent powder law introduced by Asaro [32] was used in the present study. The resolved shear strain rate (RSSR) $\dot{\gamma}^{(\alpha)}$ on a slip system is assumed to be related to the resolved shear stress $\tau^{(\alpha)}$ by power law as follows:

$$\dot{\gamma}^{(\alpha)}=\dot{\gamma}_0^{(\alpha)} sgn\,(\tau^{(\alpha)}) \left|\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}}\right|^n \text{ for} |\tau^{(\alpha)}| \gg \tau_c^{(\alpha)} \tag{1a}$$

$$\dot{\gamma}^{(\alpha)}=0 \text{for} |\tau^{(\alpha)}| < \tau_c^{(\alpha)} \tag{1b}$$

and

$$sgn\,(x) = \begin{cases} -1, & x < 0 \\ 1, & x \geq 0 \end{cases} \tag{1c}$$

where $\dot{\gamma}_0^{(\alpha)}$ is the reference value of the shear strain rate, which is taken to be a constant for all slip systems, and n denotes the rate sensitive exponent. Both $\dot{\gamma}_0^{(\alpha)}$ and n are the material characters. $\tau_c^{(\alpha)}$ is a variable used to describe the current strength of the slip system α, also known as the critical resolved shear stress. The rate of increase of the critical resolved shear stress $\tau_c^{(\alpha)}$ is expressed by:

$$\dot{\tau}_c^{(\alpha)}= \sum_{\beta=1}^{N} h_{\alpha\beta}\dot{\gamma}^{(\beta)} \tag{2}$$

where the matrix $h_{\alpha\beta}$ contains the hardening moduli for each slip system. $h_{\alpha\alpha}$ ($\alpha = \beta$) is known as the self-hardening while $h_{\alpha\beta}$ ($\alpha \neq \beta$) is known as the latent hardening.

The hardening models have been extensively studied by Taylor [34,35], Hutchinson [36], Peirce et al. [37], and Bassani and Wu [38,39]. Many comparative studies of the hardening models mentioned above have been carried out to simulate the finite and large strain deformations [40–43]. It has been found that Bassani and Wu model could reflect the hardening of face-centered cubic (FCC) crystals more exactly and was the best texture predictor. Recently, the Bassani and Wu hardening model has been successfully employed to predict the deformation behaviour and texture evolution in the large strain equal channel angular pressing process [44,45] and rolling [33,46]. Therefore, in this study, the hardening model of Bassani and Wu was adopted. Their expression for self and latent hardening are expressed as:

$$h_{\alpha\alpha} = \left[(h_0 - h_s) sech^2 \left(\frac{(h_0 - h_s)\gamma^{(\alpha)}}{\tau_1 - \tau_0}\right) + h_s\right]\left[1 + \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N} f_{\alpha\beta} tanh\,(\frac{\gamma^{(\beta)}}{\gamma_0})\right] \tag{3a}$$

$$h_{\alpha\beta}=q h_{\alpha\alpha} \alpha \neq \beta \tag{3b}$$

where q is a latent hardening parameter, γ_0 is the reference value of slip, γ is the resolved shear strain, τ_0 is the initial critical resolved shear stress, τ_1 is the breakthrough stress where large plastic flow begins, h_0 is the hardening modulus just after the initial yield, h_s is the hardening modulus during easy glide and $f_{\alpha\beta}$ represents the magnitude of the strength of a particular slip interaction between two slip systems α and β. The factor $f_{\alpha\beta}$ depends on the geometric relationship between two slip systems. There are five constants for $f_{\alpha\beta}$, namely α_1 (no junction), α_2 (Hirth lock), α_3 (coplanar junction), α_4 (glissile junction) and α_5 (sessile junction).

2.2. Finite element model

A three-dimensional finite element model was constructed to simulate the deformation process of HPT, as illustrated in Fig. 1. The disk-shaped sample with 10 mm of diameter and 0.8 mm of thickness was assumed as deformable body, while the upper and lower HPT anvils were set to rigid bodies. The sample was meshed into 23,600 elements and 26,895 nodes in total and C3D8R elements were applied. Enhanced hourglass control was used, which provides an increased resistance to the hourglassing problem and a more accurate displacement solution. Two coordinate systems, global system C_g (X, Y, Z) and local system C_l (R,θ, Z), were established, as shown in Fig. 1(b). The local R, θ, and Z axes represent the radial direction, shear direction or tangential direction, and shear plane normal or axial direction at a given location in the global system, respectively. The global coordinate system was used in the simulation, while the local coordinate system was used in the post-processing data analysis. During the simulation, the lower anvil was fixed. The rotation boundary condition along the Z axis was applied to the upper anvil while the other freedoms of the

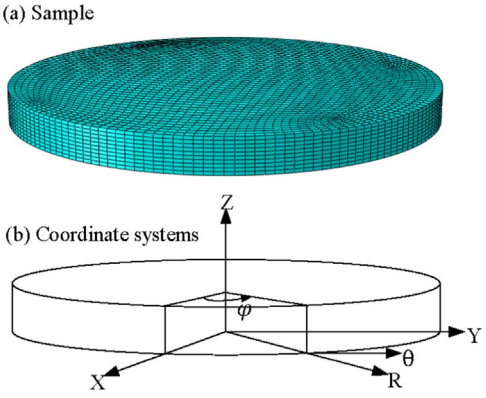

Fig. 1. Three-dimensional HPT model.