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A Dislocation-Based Model Considering Free Surface Theory Through HPT Process: Nano-Structured Ni

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Abstract. *In this study, a dislocation-based model is presented for investigating the evolution of microstructure and mechanical properties of thin films during a wide range of straining. The model is applied to the High Pressure Torsion (HPT) process of thin nickel disks that provides valuable information on the evolution of material parameters during deformation. The model considers a free surface theory for thin films and can explain the size effect phenomenon in agreement with previous reported trends in literature.*

Keywords: *Dislocation-based model; Free surface theory; Size effect phenomenon; HPT; Thin film.*

INTRODUCTION

One of the most lucrative approaches of material processing is Severe Plastic Deformation (SPD) technique which can synthesize fully dense, contamination free nanostructured material with improved strength and toughness. The optimized properties of processed materials by SPD attracted the considerable attentions of scientific committees during last years. Reviewing recent publications shows that although numerous researchers have investigated the theoretical and experimental aspects of bulk and sheet SPD processes [1,2], there is not any modeling work on investigation of the behavior of thin films during SPD processes. Therefore, the aim of this study is modeling an investigation of the microstructure evolution and mechanical properties development of thin film materials during the SPD process. This attempt leads to a model which is able to explain the size effect phenomenon in thin films during large strains.

Generally, the term 'thin film' is attributed to samples which are at least in one dimension under 1 mm [3]. The value of 1 mm is not an absolute value; it decreases when materials with smaller microstructure size are investigated. Advances in small-scale technologies have triggered a remarkable growth in the usage of these parts in micro system technologies, micro electro mechanical systems and micro surgical tools [3,4]. However, within all SPD processes, only the High Pressure Torsion (HPT) method can be used as a micro-SPD process to improve the mechanical properties of thin films. HPT technique, where a thin disk-shaped sample is compressed using a rotating plunger at pressures of several GPa, is an alternative technology for producing nanocrystalline metals. The simultaneous application of large compressive and shear strains results in the formation of very small grain sizes [5]. For example, Yang [6] reported the effectiveness of HPT process on refining the microstructure of nickel thin disks.

It has been demonstrated that the behavior of thin film materials is different from common materials. For common materials, the strength is not dependent on the sample thickness or, in some cases, it is increased due to sample thinning [7]. However, this trend is reversed for thin films, and their strength is proportional to their thickness [3,7-9]. Two major theories have been presented to explain this behavior; the strain gradient theory and the free surface theory. The strain gradient theory suggests that non-homogeneity of deformation at the microscale leads to

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observation of the mentioned behavior in thin films [10]. However, the size effect in the pure tension test of thin films [3] cannot be associated with the strain gradients, as deformation remains homogeneous up to the onset of necking. The second theory considers the surface of samples as dislocation annihilator face and predicts that increasing the ratio of surface to volume of films, (η), leads to strength dropping [4,11,12]. Although the second theory is usually neglected, there are some examples that prove the reliability of this theory. For example, it has been shown that interface constrained samples exhibit lower size dependence than that of free standing samples [13]. In addition, it has been reported that the strength of passive or coated films with amorphous layers is nearly independent of their thickness [11,12]. These examples show that elimination of the free surface removes or decreases the intensity of the size effect phenomenon. Although these examples describe the importance of the second theory [4], effective implementation of this theory to the models which are able to predict microstructure or mechanical property evolution during deformation has been neglected in prior studies. The aim of this work is to emphasize the need for considering the free surface theory besides the strain gradient theory whenever size effect phenomenon is discussed.

In an attempt similar to that undertaken in this paper, Molotnikov et al. [3] presented a model that considers material in two parts, a soft (non-hardening) part at the surface and a hard part of the center. Considering this assumption, they investigated the mechanical behavior of thin films during straining. Although the results of this model were in good agreement with the experimental data, there are some problems in this model that decrease its scientific reliability. For example, considering such a soft surface is not a realistic assumption and in the case of applying this model to processes which include surface shear straining like HPT process, the whole strain would localize at the surface of sample.

The most famous model, applicable to SPD is the ETMB (Estrin, Toth, Molinari, Brechet) model. This model was used by Molotnikov et al. [3], however, it includes several mathematical coefficients that decrease the scientific value of the model. Thus in the present study, considering the deficiencies of earlier works, a physical-metallurgical-based model is proposed for modeling the SPD of thin films, which considers the surface of samples as an infinite sink for dislocations. It is shown that the model can predict the evolution of the microstructural and mechanical parameters of materials in good agreement with the experimental data and also it can explain the size effect phenomenon consistent with the earlier reports in literature.

In this paper, after describing the model, it is applied to the HPT process of thin nickel disks and the modeling results are compared with the experimental results of XRD carried out by Yang [6]. Also, the ability of the model in describing the size effect phenomenon of thin films is discussed through computing the strength and work hardening intensity of materials with different η values.

MODEL DESCRIPTION

In this section, a description of proposed model for investigating the behavior of thin films under SPD processes is presented. In the model, similar to other models on SPD [14,15], the material is considered to be broken up into two distinct, but dependent, phases: cell interiors with a relatively low dislocation density, and cell walls with a higher dislocation density. The dislocation densities in these two distinct regions are considered to be the internal variables of the model and the total dislocation density is given by a rule of mixtures in the material. In the following, the model defines the mechanisms of dislocation generation and annihilation in both phases and investigates the evolution of their dislocation densities during deformation.

Here, two phenomena are considered to increase the dislocation density in cell walls. The first is related to the migration of some dislocations from cell interiors to cell walls and the second is the activation of Frank Read sources [15]. Also, dislocation annihilation in cell walls is defined through dynamic recovery mechanisms. Therefore, regarding the works carried out in [2,15-20], the following mechanism-based equation is proposed for dislocation density evolution of cell walls:

$$(\dot{\rho})_w = \frac{6\alpha^*\dot{\gamma}_c(1-f)^{2/3}}{bdf} + \frac{\sqrt{3}\alpha^*\dot{\gamma}_c(1-f)\sqrt{\rho_w}}{fb} - \frac{\beta^* D_L \rho_w^2 \mu b^3}{K_b T}, \quad (1)$$

where ρ_w is the dislocation density in cell walls, d is the cell size, f is the volume fraction of cell walls, b is the magnitude of the Burgers vector, D_L is the lattice diffusivity, μ is the shear modulus, K_b is the Boltzmann constant and T is the absolute temperature. Also, α^* and β^* are the model parameters. The parameters $\dot{\gamma}_c$ and $\dot{\gamma}_w$ are the resolved shear strain rates in cell interiors and cell walls, respectively.

Here, the first term in represents the increasing effect of dislocations migrating from the cell interiors to the walls. When these dislocations cross the interface between the cell interiors and the cell walls, they are also expected to activate Frank-Read sources located at the interface, giving rise to the dislocation density of cell walls according to the second term. These two terms came in 1998 by Estrin et al. [15], and a very detailed explanation about derivation of these two

terms can be seen in [15]. Finally, the third term accounts for annihilation of cell wall dislocations due to dynamic recovery. It has been reported [20,21] that the main active mechanism of dynamic recovery at cell walls is climbing. This idea is mainly arisen from a high energy condition and also complex configuration of dislocations at the walls. In this model, instead of using the expression used by Estrin et al. [15], a more physical based expression is used. This expression used in previous works of the present authors [16,17], relates the rate of dislocation annihilation in dislocation walls through the climbing process to the diffusion intensity and the energy level of walls (dislocation density of cell walls). The origin of this equation can be seen in the work carried out by Rezvanian et al. in 2006 [20]. Here since the focus is on the size effect phenomenon, the detailed explanation of the derivation steps of these equations is not mentioned (for more information see [15,20]).

Previous experimental work [7,22,23] reported that the magnitude of d affects the intensity of the size effect phenomenon. Therefore, although in earlier theoretical attempts to model the size effect [3] the evolution of d during straining was not considered, in this model, d is considered to be related to the total dislocation density of material [24] as a dynamic quantity to make more accurate predictions.

For cell interiors, activation of Frank Read sources is the sole mechanism of dislocation generation [15], while three mechanisms lead to dislocation loss; dislocations migration to cell walls [15], dynamic recovery through cross slip [20] and annihilation of dislocations at the free surface which should be considered for thin films, specifically [4]. The last mechanism is not important for normal materials, but in the case of thin samples, it is meaningful to consider it. Here as a first step, the expressions describing three first processes are reviewed briefly, since they are not a novelty of this work and come from previous work [15,20]. So neglecting the case of thin samples, we would have the following equation for describing the dislocation density evolution of cell interiors.

$$(\dot{\rho})_c = \frac{\zeta^* \dot{\gamma}_w \sqrt{\rho_w}}{\sqrt{3}b} - \frac{6\alpha^* \dot{\gamma}_c}{bd(1-f)^{1/3}} - \frac{2\varsigma^* \nu_0 \sqrt{\rho_c}}{l} \left[\exp\left(-\frac{Q(1-\alpha b\sqrt{\rho_c})}{K_b T}\right) - \exp(-\frac{Q}{K_b T})\right], \quad (2)$$

where ν_0 is the attack frequency, l is the length of a potential site for cross slip, Q is the activation enthalpy of cross-slip, α is a factor that weights dislocation interactions and ζ^* and ς^* are the model parameters.

Here, the first term in Equation 2 describes the influence of Frank Read source activation and the two following expressions describe the effect of two phenomena which led to dislocation decreasing in cell interiors. The second term in Equation 2 introduces the effect of dislocation migration from cell interiors to cell walls. This term is equivalent to the first term in Equation 2. Also, the third term in Equation 3 is describing dislocation density decreasing due to dynamic recovery which in the case of cell interiors has been attributed to the cross-slip phenomenon [20,21]. The main supporter for this idea is related to the low energy condition of cell interiors which is not enough for high rate climbing. Again, since these equations and their coupling have been introduced in previous works, more detailed discussion about their foundations has been skipped and they can be seen in [15,20].

Anyway, here a new expression is added that describes the effect of a free surface and can have more relevant effect in a case of thin films. Since this term is introduced in this work, more details about the steps of its derivation are mentioned. The term would have a decreasing effect on the dislocation density of cell interiors and is derived by considering the free surface of material as an infinite sink for dislocations.

It can be considered that the effect of a free surface penetrates until a specific depth of material that is proportional to the dislocation velocity in a direction perpendicular to the film surface. Therefore, there is a surrounding volume where located dislocations are attracted to the surface for annihilation. As a consequence, the following relation can be presented for dislocation annihilation during the time interval of dt on the film surface:

$$d\rho_c^{\text{free surface}} \propto -\rho_c S \left(\frac{4}{\pi^3} V_d\right) dt, \quad (3)$$

where ρ_c is the dislocation density of cell interiors, S is the surface area of the film and V_d is the velocity of dislocations in cell interiors. Therefore, considering the Orowan relation [15] and the ratio between the surface and volume of film, η, the following equation describes the evolution of cell interior dislocation density due to the free surface effect:

$$(\dot{\rho})_c^{\text{free surface}} = -\xi^* \eta \frac{4\dot{\gamma}_c}{\pi^3 b(1-f)}, \quad (4)$$

where ξ^* defines the intensity of penetration of the free surface effect. So, the mechanism-based equation for the dislocation density evolution of cell interiors is:

$$(\dot{\rho})_c = \frac{\zeta^* \dot{\gamma}_w \sqrt{\rho_w}}{\sqrt{3}b} - \frac{6\alpha^* \dot{\gamma}_c}{bd(1-f)^{1/3}} - \frac{2\varsigma^* \nu_0 \sqrt{\rho_c}}{l} \left[\exp\left(-\frac{Q(1-\alpha b\sqrt{\rho_c})}{K_b T}\right) - \exp\left(-\frac{Q}{K_b T}\right)\right] - \xi^* \eta \frac{4\dot{\gamma}_c}{\pi^3 b(1-f)}. \quad (5)$$

As mentioned, η is the ratio between the free surface and the volume of the sample. In the case of the HPT sample, the η is derived by considering:

$$\eta = \frac{\text{Surface of disk } (\text{m}^2)}{\text{Volume of disk } (\text{m}^3)}.$$

For showing the effect of a free surface in the discussion section, the theoretical values of η between 0 (coated sample) and 12 m^{-1} have been considered. The above equation explains interestingly the effects of the sample and microstructure sizes. By increasing the size of the sample which would mean mainly increasing the thickness of the sample, the value of η would decrease and cause the decrease of the free surface theory effect on the behavior of the material. Also, by applying the deformation, the structure size of the material is decreased and the mutual changes in the volume of cell interiors and cell walls due to deformation cause a decrease in the value of the f parameter [15-17]. This would cause a decrease in the $\frac{1}{(1-f)}$ term and a decrease in the intensity of the free surface theory. Both concepts are compatible with the foundation of the free surface theory in thin films and would suggest that the maximum thickness of a sample that can be counted as a thin film is a function of its microstructure size.

Thus by solving the above differential equations, it is possible to describe the microstructure evolution of thin films during SPD processes.

In this paper, considering the mechanical analysis proposed by Zhilyaev et al. [25] and the Taylor crystal plasticity model [15], the above differential equations are solved numerically and simultaneously for the HPT process for a pure nickel thin disk. Then, the dislocation density and cell size of the processed nickel are investigated. Also, considering the existing relations between dislocation density and other parameters, the strength, microstrain and misorientation of the processed nickel are anticipated. The used material parameters and also the size of samples are summarized in Table 1.

RESULTS AND DISCUSSIONS

Microstructure Evolution

The predicted microstructural parameters of processed nickel by HPT are presented in Figure 1.

During preliminary straining, the intensity of dynamic recovery is negligible and hence dislocation density growth, or in other words, work hardening is the prominent behavior of the material. However, more deformation provides a high driving force for softening processes and increases the intensity of dynamic recovery which leads to a decrease in the rate of work hardening. Therefore, as can be seen, the dislocation density is increased sharply during initial HPT revolutions and reaches a saturated value through the following revolutions. It should be noted that the predicted results are in agreement with the experimental data reported by Yang and Welzel [28]. Also, the described trend is repeatedly observed in earlier experimental works on HPT of other materials [24,29].

In addition, the model predicts a quick cell size refining during the first HPT revolution and a nanostructured material is achieved in the following revolutions. As seen in Figure 1, the agreement between modeling and experimental cell sizes is remarkable.

Table 1. The values of material parameters and sample geometry [2,6,15,18-20,26,27].

Parameter	Symbol	Value
Sample diameter	D_{disk}	1000 μm
Sample thickness	t_{disk}	300 μm
Magnitude of Burgers vector	b	24.9 nm
Lattice diffusivity coefficient	D_L	1.55×10^{-20} m^2s^{-1}
Shear modulus	μ	79 GPa
Attack frequency	ν_0	10^9s^{-1}
Activation enthalpy of cross-slip	Q	$8.651757582 \times 10^{-19}$ J
Length of a potential site for cross slip	l	1000 b
Initial dislocation density in cell interiors	ρ_{c_0}	10^{12} m^{-2}
Initial dislocation density in cell walls	ρ_{w_0}	10^{13} m^{-2}
Cell size	d	$\frac{[2.756+(5.957-2.765)\exp(-9.6\varepsilon)]}{\sqrt{\rho_{\text{Total}}}}$
Volume fraction of cell walls	f	$0.08 + (0.25 - 0.08)\exp(-0.3216\varepsilon)$

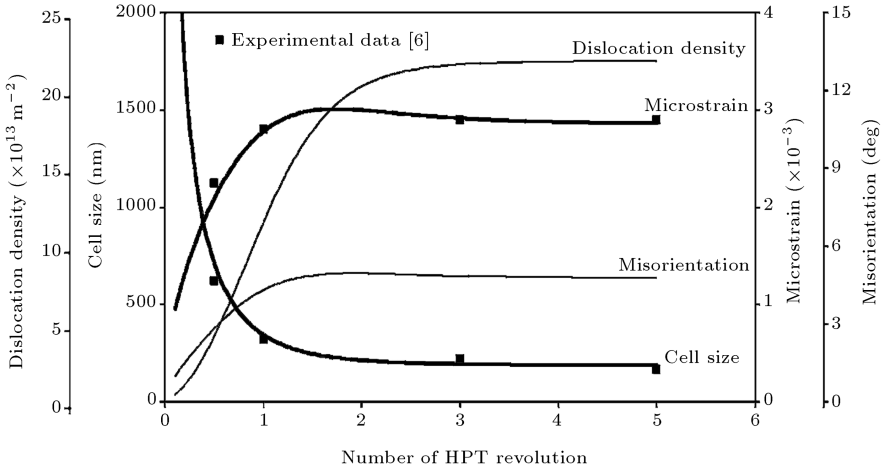

Figure 1. The evolutions of microstructural parameters of nickel during HPT process [6].

Considering the relation between dislocation density, cell size and microstrain [6], the magnitude of the microstrain of processed nickel is presented as a function of HPT revolution. The predicted trend for microstrain evolution involves four stages: intensive increasing, temporary saturation, little dropping and prominent saturation. Initial deformation and work hardening increase the density of lattice defects and lead to intensive microstrain rising. However, dynamic recovery causes the density of lattice defects, and thus the microstrain value to decrease [6]. Therefore, competition between microstrain rising due to work hardening and its decreasing due to dynamic recovery leads to creation of the observed trend for microstrain evolution. Also, as can be seen, the predicted values for microstrain are extremely consistent with the experimental data of processed nickel by HPT [6].

Furthermore, the calculated angle for misorientation of low angle grain boundaries [30] shows the usual trend observed during SPD processes [31]. It should be noted that the angles presented here are compatible with the experimental data presented by Zhilyaev et al. [25] which were undertaken on HPT of nickel.

Size Dependence Phenomenon

During recent years, some authors have studied the effect of film thickness on their mechanical response during small deformation [3,7-9]. However, there are no studies on the investigation of size effect during large strains. Hence in this section, assuming a wide strain range, the effect of specimen thickness or, in other words, the effect of its η value, on the evolution of strength and work hardening intensity is discussed using the predictions achieved from the presented model explained in the previous sections. To do so, a sample that is coated with an amorphous layer, which eliminates the effect of free surface, is considered as a reference sample and the strength evolution of samples with different η values are compared with its strength evolution (see Figure 2). So, a normalized strength is defined through the ratio between the strength of each specimen and the strength of the coated sample.

Consistent with earlier reports [3,7,8], the model predicts that by increasing the η values of films, their strengths are dropped, because the specimen with a high η value provides much more surface for dislocation annihilation and strength softening. The more interesting fact is that the model anticipates a higher difference between strengths of samples in small magnitudes of strains rather than in large strains. This trend can be evaluated considering two aspects. First, straining refines the microstructure and increases the number of grains that are placed in the film thickness. This phenomenon, as described in several experimental reports [7,22,23], decreases the intensity of free surface

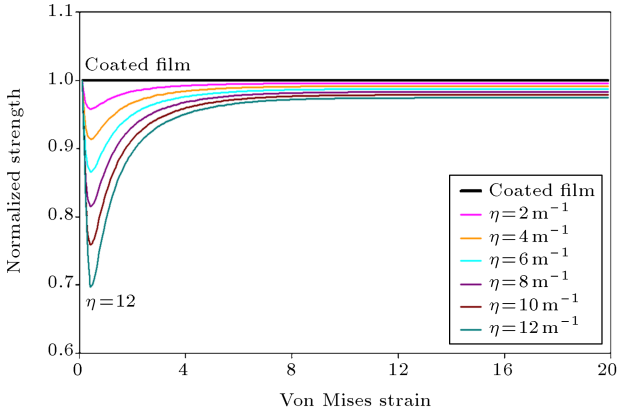

Figure 2. Normalized strength of specimens with different η values versus strain (normalized coordinate is defined in the text).

effect. Accordingly, this idea could be conceived that the model truly predicts that the maximum thickness of sample that can be counted as thin film would decrease by decreasing the microstructure size due to straining. Physically, it means that by decreasing the microstructure size, there are more barriers preventing dislocations from reaching the free surface and decreasing the size effect phenomenon. Second, since during initial stages of straining, the intensity of dynamic recovery is negligible, so operation of a secondary softening mechanism, such as free surface softening is more obvious than that under the larger deformation condition where a more powerful softening mechanism (dynamic recovery) is active. Therefore, it is acceptable that the intensity of a free surface effect is decreased with increasing the magnitude of deformation. It should be noted that, although this trend has been reported in earlier experimental work (For example see [8]), none of the prior modeling work could describe it.

Figure 3 shows the effect of the η value of a sample on the intensity of work hardening (n value in the Hollomon equation).

Although earlier experimental work [8] has investigated the effect of specimen size on the work hardening intensity of thin films, this event has not yet been investigated through modeling work. As can be seen in Figure 3, the model predicts a weak work hardening for the samples with high η values during a low magnitude of deformation. This trend has been reported in the work carried out by Michel and Picart [8]. However, as shown in the figure, the intensity of the work hardening of samples with high η values in large strains is more than that of the coated sample or samples with lower η values. As mentioned in earlier sections, the dynamic recovery process in large strains intensely affects the mechanical response of materials and decreases the work hardening intensity. Also, as can be seen in metallurgical texts and also

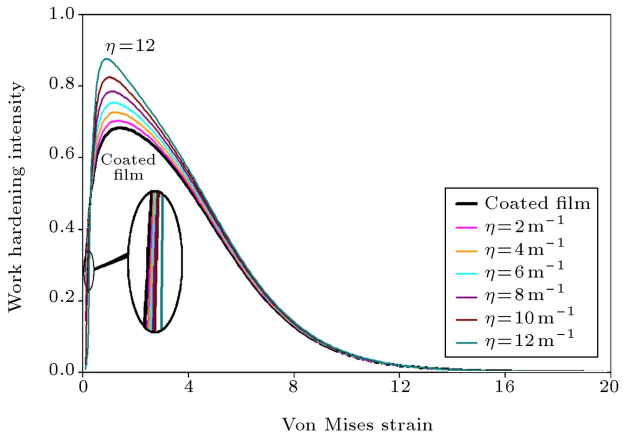

Figure 3. Work hardening intensity of specimens with different η values versus strain.

in Equations 1 and 2, the rate of recovery is strictly dependent on the dislocation density. Considering the relation between material tensile strength and dislocation density, and also Figure 2, it can be concluded that the dislocation density of samples with high η values is lower than that of samples with low η values. This condition causes a lower rate of dynamic recovery and lower work hardening intensity for samples with high η values at large strains. However, unifying the dislocation density of all samples in very large deformation causes unified work hardening intensity to be obtained.

Considering cell size as a dynamic quantity enabled us to have a lower size effect in smaller cell sizes, which is reasonable. It means by increasing the strain, the size of material structure is decreased and causes less size effect on higher strains. This idea cannot be derived by considering a constant structure size, which has been considered in previous attempts [3].

CONCLUSIONS

In this study, a physical-metallurgical-based model is proposed for investigating the evolution of the microstructural and mechanical parameters of thin films during a wide range of straining. The model takes into account geometrical dimensions of samples and considers the free surface of specimens as an infinite sink for dislocations. The proposed model is applied to the HPT process of a nickel thin disk and the evolution of its microstructural and mechanical parameters is presented. Comparing the results of the model with earlier reports on the HPT of nickel shows good agreement. Also, the model investigates the size effect phenomenon of thin films through the concept of the ratio between their surface and volume (η) during small and large strains. This case has not been investigated in earlier works. The modeling results show that during small deformation, the magnitudes of strength and the intensity of the work hardening of samples with high η is lower than that of the coated sample or samples with low η, as observed in earlier experimental work. However, the model predicts that more deformation causes a decrease in the difference of strength between samples with different η values. Also, the modeling results anticipate intensive work hardening for samples with high η in large strains, which eliminates the difference between the strength of the samples.

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