Statistical dislocation activation from grain boundaries and its role in the plastic anisotropy of nanotwinned copper

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Abstract

In this work, we explore the microstructural properties that give rise to the plastic anisotropy observed in columnar-grained, nano-twinned Cu. A statistical model for randomly varying source lengths within the grain boundaries of the nanostructure is developed. The model is used to calculate a corresponding critical resolved shear stress for emitting dislocations within a twin lamella on slip systems lying either parallel or inclined from its twin boundary. By incorporating this model into a 3D crystal plasticity finite element model, we can link texture and slip patterns within the twin lamella to anisotropy in the plastic deformation behavior. The model achieves good agreement with flow stress strain evolution and yield data collected over many studies. We show that reducing twin thickness can increase plastic anisotropy as a result of the increase in mean stress to emit dislocations. It is also found that finer twins can lower strain hardening as a consequence of a lower statistical variation in the emission stress.

Keywords: crystal plasticity, texture, size effects, strength, interface

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1. Introduction

Metals with nanoscale twins have been under the spotlight in the materials community for many years because of their unique properties and great potential in nanoscale devices. Unlike nanocrystalline (NC) metals, which possess ultrahigh strength and hardness but suffer from very limited ductility and strain hardening [1], nanotwinned (NT) metals can exhibit excellent strength while maintaining substantial ductility [2-4]. In addition, NT metals possess other desirable properties, such as outstanding thermal stability [5, 6], electrical conductivity [7, 8] and fatigue resistance [9, 10]. One of the fundamental reasons that NC and NT metals exhibit markedly different mechanical behavior resides in the different characteristic length scales they possess. NC metals only have one characteristic length scale, i.e., the nanoscale grain size. In contrast, NT metals have two length scales: grain size and twin thickness [11]. Similar to grain boundaries (GBs), twin boundaries (TBs) serve as effective barriers to dislocation motion [12, 13]. The small, nanoscale twin thickness leads to a high density of TBs, which confines dislocations within the twin lamellae and causes dislocation pile-ups, giving rise to significant strengthening.

Among the NT metals, copper (Cu) has been one of the most intensely researched. NT Cu has been categorized as equiaxial-grained [12] and columnar-grained [14]. The major difference between these two NT types is the orientation of the nanoscale twins. In equiaxial-grained NT Cu, twins are randomly oriented based on the orientation of each grain. While in columnar-grained NT Cu, the nanotwins boundaries are highly oriented about the NT growth direction. Due to this preferential crystallographic orientation, this type of NT Cu can be expected to exhibit strong plastic anisotropy when subsequently deformed [11, 15, 16]. You et al.[16] report that both yield strength and strain hardening of columnar-grained NT Cu depend on the loading orientation with respect to the TB. Their samples were tested at room temperature and applied strain rates of 0.001/s. When the loading orientation is perpendicular to the TBs, the yield strength is the highest, but strain hardening is negligible. When loaded parallel to the TBs, the yield strength was lower and strain hardening higher. When the loading axis is inclined 45° to the TBs, the NT Cu samples demonstrated the lowest yield strength and significant strain hardening. In contrast, equiaxial-grained NT Cu exhibits near plastic isotropy because of the randomly oriented twin layers [17].

Thus far, most computational material modeling efforts have focused on the deformation behavior of equiaxial-grained NT Cu [18-24]. The underlying mechanisms giving rise to the anisotropic properties exhibited by columnar-grained NT Cu have received noticeably less attention. As an exception, recent molecular dynamics (MD) simulations were applied to study dislocation nucleation and motion in deformed polycrystalline columnar NT Cu [16]. They revealed that GBs were the favorable dislocation nucleation sites and both partial and full dislocations were observed during deformation. It was also observed that different loading directions can be associated with distinct modes of dislocation propagation and interactions with the TBs. Borovikov et al. performed large-scale MD simulations on the effect of texture on the yield and peak stresses in columnar-grained nanotwinned Ag and Cu [25, 26]. Their simulation results suggested that, in NT face-centered cubic metals, the strength is determined primarily by the cooperation or competition between two major factors: the magnitude of the Schmid factors for the available slip systems and the effectiveness of grain boundaries (and their triple-junctions) in generating dislocations. However the short time and length scales characteristic of these techniques prevent them from examining the combined effects of texture evolution and dislocation activity in a rate regime consistent with laboratory tests (room temperature, quasi-static rates). Spatially resolved crystal plasticity (CP) finite element models are well suited for modeling the effects of texture evolution, crystallographic elastic and plastic deformation, and heterogeneous stress fields with plastic anisotropy realized in standard, ambient mechanical tests [27, 28]. However, an inherent drawback of most CP based techniques is that they use hardening laws based on homogeneous slip [29, 30]. This limitation would make them not applicable for understanding the behavior of nanostructured metals in which individual dislocations can be resolved and the amount they slip is dictated by the grain size and twin thickness. In an attempt to overcome this constraint, in prior work, we developed a constitutive model for NC metals in which plasticity occurs by discrete slip events activated statistically from grain boundaries [31]. The model was incorporated into a crystal plasticity finite element model for NC Ni in order to understand grain size effects on yield strength. It predicted the emergence of Hall-Petch like behavior in the nanoscale regime in agreement with several experimental NC Ni hardness studies [32-35].

The goal of this work is to develop a CP-based model that can simulate the statistical emission of dislocations from grain boundaries in NT materials and use it to understand the

effect of the length scales characteristic of columnar-grained NT materials on plastic anisotropy. Within this model, slip occurs within each twin lamella by discrete slip events on slip planes that are either parallel and non-planar to the twin boundary and whose range is respectively restricted by the grain size and twin thickness. With it, we explore the relative effects of twin thickness, grain size, and initial texture on the plastic anisotropy in yield strength, flow stress, and strain hardening of NT Cu. The model indicates that finer twin thicknesses can increase the plastic anisotropy of NT Cu, by virtue of an increase in the mean stress to emit dislocations. The analysis also suggests that lower statistical variation in the emission stress with decreasing twin thickness leads to a reduction in strain hardening.

2. Deformation model of NT material

In this section, a CP-based mechanics model is presented for columnar-grained NT materials. It is a multi-scale model built upon a crystal plasticity finite element (CPFE) framework. At the highest level is the polycrystal, which is idealized as an aggregate of equal sized, equal shape grains of diameter D . At the grain scale, the twins can be resolved. Every grain is laminated by multiple NTs, each separated by a (111) twin plane and possessing the twin-matrix orientation relationship. Among the grains, the NT (111) twin planes differ in orientation with respect to the sample, according to a specified texture. At the finest scale, within an individual lamella, plastic deformation is mediated by dislocation motion, where dislocations emanate exclusively from the GBs and may glide on multiple slip systems.

To this multiscale NT model microstructure, a load is applied, and as strain increases, the crystallographic orientations are permitted to evolve. The model outputs examined are multiscale in nature, ranging from the macroscopic flow stress, to microstructural texture evolution, and to the predominant modes of slip within individual lamellae, as a function of D and twin thickness λ .

2.1 *Crystal plasticity finite element*

Crystal plasticity finite element (CPFE) method is used to relate the local elastic and plastic constitutive response to the macroscopic polycrystalline response. This calculation accounts for interactions among grains and twins. The stresses amid the twins can vary and their stress states can deviate from the macroscopic stress state. The individual twin lamella may reorient with slip from their initial twin-matrix relationship and hence the overall material texture can evolve.

In order to incorporate the constitutive equations into the CPFE simulation, a user-defined material subroutine (UMAT) developed by Marin et al. is implemented into Abaqus [36-38]. The UMAT is based on a rate-dependent, elasto-viscoplastic constitutive model, which explicitly accounts for elastic and plastic anisotropy, crystallographic slip, grain rotation, and texture evolution [36-38]. A full description of the constitutive equations and the two-level iterative scheme used to solve them can be found in [37, 39]. The key modification made here concerns the plastic part of the velocity gradient, $\mathbf{L}^p$. It accounts for the plastic deformation generated by dislocation glide on crystallographic slip planes and is taken to be the summation of the plastic flow over all slip systems as

$$\mathbf{L}^p = \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{b}^{\alpha} \otimes \mathbf{n}^{\alpha} \quad (1)$$

where $\mathbf{b}^{\alpha}$ and $\mathbf{n}^{\alpha}$ are the slip direction and slip plane normal on slip system α and $\dot{\gamma}^{\alpha}$ is the shear strain rate on slip system α . The form of $\dot{\gamma}^{\alpha}$ is adapted for statistical emission of dislocations from grain boundaries and is described in Sections 2.2 and 2.3.

The NT material model is comprised of an aggregate of grains of diameter D aligned in columns. Each grain consists of N parallel twin lamellae that are λ thick. Adjacent nanotwins within the grain have the twin-matrix orientation relationship and the interface plane corresponds to a $\{111\}$ twin boundary (TB). The top and bottom faces of the grain are grain boundaries and the distance between them is thus $N\lambda$. The geometry of the FE model corresponding to this NT microstructure is shown in Figure 1 as well as the x-y-z coordinate system. An element in the mesh is a twin lamella with dimensions in x, y, and z of $D \times D \times \lambda$. Without loss of generality, all grains consist of the same number N of lamellae and in the calculations that follow, we set $N = 8$. The polycrystal model, therefore, contains 1000 grains and 8000 lamellae (elements).

The N lamella belonging to the same grain share the same (111) boundary normal and have the twin-matrix orientation relationship. However, the crystallographic orientation of each NT grain can vary from grain to grain. For the starting model microstructure, the common (111) TB of each grain is assigned a crystallographic orientation from a measured or hypothetical texture. For most of our calculations here, the model initial texture corresponds to one naturally found in as-deposited NT materials, like the one given in Figure 2, taken from You et al. [16]. As shown, most of the (111) twin boundary planes of the lamellae are oriented within 25° of the sample z-axis and the other axes (110) and (112) are randomly oriented from grain to grain.

It must be noted that the CPFE elements correspond to nanotwins in dimension but not necessarily in crystallography. The N elements belonging to the same grain share the same (111) boundary normal and have the twin-matrix orientation relationship as shown in Figure 1(c). However, due to the spread in the TB orientation with respect to the growth direction (the z-axis in Figure 1(b)), the boundary between finite elements is not necessarily aligned with the (111) TB between twin lamellae.

2.2 Size-restricted boundary sources for dislocations

Figure 3 shows the model geometry of an individual twin lamella. The cross section of a twin lamella is modeled as a hexagon. The shortest distance D between two opposing facets of the hexagon corresponds to the grain size D . The six sides of the twin lamella are grain boundaries (GBs). Each lamella has six grain-boundary junctions (GBJs), where two neighboring grain boundaries meet.

In this model, plasticity of the twin lamellae is mediated by dislocations on the 12 fcc $\{111\}\langle 110 \rangle$ slip systems. Prior to deformation, the TB planes correspond to $\{111\}$ planes. Thus, in every twin lamella, the common (111) glide plane of three of the 12 slip systems will be parallel to the TB plane and those of the remaining nine slip systems will lie inclined to the TB plane. We will distinguish the former as boundary parallel or *b-parallel* planes and those of the latter as boundary inclined or *b-inclined* planes.

In each lamella, dislocation activation is classified as heterogeneous, meaning dislocations emanate from a pre-existing defect. In this model, the source defects are double-pinned dislocations of length L . We further assume that in the confined nanoscale dimensions of NTs, the number of such sources within the twin interior and in the flanking coherent twin boundaries is negligible compared to the number lying in the GBs and GBJs. Therefore, dislocation sources will lie exclusively in the GBs and GBJs.

The critical resolved shear stress (τ_{CRSS}) for activating the source of length L is given by [40, 41]:

$$\tau_{CRSS} = \frac{A}{2\pi} \frac{\mu b}{L} \log \left(\frac{L}{\omega \cdot r_0} \right), \quad (2)$$

which is the stress to bow out the dislocation and have it reach an unstable configuration of a half loop of radius $L/2$. Parameter A is a constant of order unity, μ is the effective shear moduli of

the crystal, r_0 is the core radius of the dislocation, and ω is the interaction parameter that takes into account elastic interactions with the more distant portions of the same dislocation line [41]. For the Cu material studied here, $r_0 = 5b$ [42], $b = 0.256$ nm and $\mu = 48.3$ GPa [43]. In addition, $A = 1.0$ and $\omega = 2.4$ can make a good prediction on experiment results as shown in Figure 6.

The activation threshold τ_{CRSS} is assumed to be greater than the stress to propagate the dislocation across the grain unhindered. As the dislocation propagates, its width w would expand to a length equal to or greater than its source length L . As this propagation stress would scale as $\log(w)/w$ scaling [14], then it follows that it is harder to emit the dislocation than propagate it through the lamella.

Within the GBs and GBJs, source lengths L will vary statistically in length and orientation. The minimum length L_{min} is set to $(e \cdot \eta \cdot r_0)$, where e is the base of the natural logarithm and η is a factor that guarantees that shorter sources need higher activation stresses, which is $\eta = 1.25$ in the present study. To serve as a source for a given slip system, the dislocation line of the source L must lie along the intersection line between the plane of the slip system and the grain boundary plane. The largest possible source lengths L will be limited by the dimensions of the twin lamella, which is λ thick and D wide. For a GB source, the dislocation line of the source must lie along the intersection line between the slip plane and the grain boundary. For b-parallel planes, the GB source lengths can range from the L_{min} to D . For b-inclined planes, this intersection line is bound between the two adjacent coherent twin boundaries λ . Thus the GB source length is limited by λ . Therefore, for dislocation sources on b-inclined planes, the possible source lengths range from L_{min} to $\lambda/\sin\theta$, where θ is the angle between the inclined slip plane and twin plane.

As an example, Figure 4 shows the distribution of τ_{CRSS} values from GB sources $\lambda = 20, 30$ and 50 nm. This distribution results from inserting all possible values of L into equation (2). We observe that the mean (and median) decreases and the covariance (standard deviation normalized by the mean) increases as λ increases. The increased dispersion in τ_{CRSS} with λ is a consequence of the maximum τ_{CRSS} being controlled by the minimum source length, which is L_{min} and is the same for all λ , and the minimum τ_{CRSS} being controlled by the maximum source length $\lambda/\sin\theta$, which increases with λ . Table 1 lists the median, mean, standard deviation, and coefficient of variation in τ_{CRSS} for all values of λ considered here.

A GBJ is a line where two adjacent grain boundaries of the same grain meet as shown in Figure 1. According to our idealized twin lamella geometry, this line does not intersect any b-inclined planes. However, a GBJ source could produce a dislocation on one of the b-parallel planes. For the GBJ source, each end of the source lies on one side of the junction (See Figure 1). Geometrically the length L of the GBJ sources can range from $L_{\min}$ to D . Hence, in this model, the GBJ source lengths are much less grain size-restricted than those of the GB sources. To demonstrate, Figure 5 shows the distribution of τ_{CRSS} values from GBJ sources for $D = 500$, 1500 and 3000 nm calculated by inserting all possible values of L into equation (2). We also see a grain size effect on τ_{CRSS} in Figure 5. As D increases, the distribution shifts toward lower values and the dispersion decreases. Thus, by virtue of statistical source lengths from grain boundaries, dislocation activation becomes easier (the statistical mean decreases) and less variable (the statistical dispersion decreases) as D increases. In addition, compared to the τ_{CRSS} for GB sources, the τ_{CRSS} values from GBJ sources are much lower. The parameters of these distributions are summarized on Table 1.

2.3 Dislocation kinetics

In the foregoing we described the slip systems available for accommodating deformation, the critical stresses to activate them, and the CPFE model that will relate the active slip systems to overall material response. As mentioned, the present model significantly deviates from conventional CPFE models since dislocation slip does not occur homogeneously but discretely, in finite movements dictated by microstructural length scales. Specifically, slip occurs as dislocations are activated from boundaries and glide completely across the grain unhindered to the opposing boundary, as observed in MD simulations [44-46]. The receiving GBs are assumed to fully absorb the dislocations such that pile-ups do not develop at the boundaries. Thus, in addition to limiting the maximum source length that can be emitted, the grain size also dictates the maximum amount of slip per dislocation emitted.

In this material model, boundary sources are arranged such that dislocations on all 12 $\{111\}\langle 110 \rangle$ slip systems are available to accommodate slip within the twin lamella. The GBJ sources can activate dislocations on the b-parallel planes and the GB sources can activate dislocations on the b-inclined planes.

The value τ_{CRSS} is viewed as a threshold to emission. When the RSS in a slip system is lower than its assigned τ_{CRSS} , a dislocation is pinned either at the GBJs or GBs and is unable to propagate. Under such circumstances, the slip system is inactive and the plastic shear rate is zero. This case is fulfilled numerically by making the shear strain rate $\dot{\gamma}^\alpha$ extremely small in the CPFE model.

When RSS reaches or exceeds the assigned τ_{CRSS} , the local stress is considered sufficiently high for the dislocation to unpin and propagate across the twin lamella, and thus the slip system becomes active. The following kinetic equation is adopted to calculate the shear strain rate in an active slip system:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left[\frac{|\tau^\alpha|}{\tau_{CRSS}} \right]^{\frac{1}{m}} \text{sign}(\tau^\alpha) \quad \tau^\alpha > \tau_{CRSS}, \quad (3)$$

where $\dot{\gamma}_0$ is a reference shear strain rate, τ^α is the RSS in slip system α , τ_{CRSS} is the CRSS for this particular slip event randomly sampled from the τ_{CRSS} distribution, and m is a strain-rate sensitivity exponent.

MD simulations have shown that changes in the GB structure can accompany the emission of dislocations from GBJs or GBs [47, 48]. With such structural alterations, source lengths and hence τ_{CRSS} would be expected to change after each dislocation emission. Within our model this phenomenon is captured by randomly assigning a new τ_{CRSS} value from the corresponding τ_{CRSS} distribution to a slip system for every new slip event. Knowing when a new slip event begins requires knowing when the previous one ends. The completion of a discrete dislocation slip event can be determined from the shear rate and the shear strain accumulated as a single dislocation glides from one end of the twin lamella to the other $\gamma_{discrete}$. Due to geometry, $\gamma_{discrete}$, would differ for b-inclined and b-parallel slip and can be calculated via [31, 49]:

$$\gamma_{discrete} = \begin{cases} \frac{b}{D} & \text{for slip systems on } b - \text{inclined slip planes} \\ \frac{b}{\lambda} & \text{for slip systems on } b - \text{parallel slip planes} \end{cases} \quad (4)$$

where b is the magnitude of Burgers vector for Cu, D is grain size, and λ is twin lamella thickness.

Within a twin lamella, several dislocations may be gliding on the same slip system but separate atomic planes. In the calculations that follow, for a given twin lamella, we allow for activation of multiple dislocations belonging to the same slip system and within the same time increment¹.

2.4 Investigation into NT size effects and plastic anisotropy

The NT material model presented above has two main microstructural length scales, D and λ , that can affect the macroscopic deformation response by directly affecting dislocation emission and propagation in two ways. First, the grain size D affects τ_{CRSS} for new dislocations on the b-parallel slip planes, while the twin thickness λ influences τ_{CRSS} for new dislocations on the b-inclined planes. Second, D and λ also limit the extent of glide on the b-parallel and b-inclined planes, respectively.

From this model, we can also expect at least three main independent sources of plastic anisotropy. The first is texture, which can be classified as a geometric anisotropy. Second is the heterogeneous distribution of the boundary planes where dislocation sources lie. That is, dislocations are not activated homogeneously at all material points, in both the boundaries and twin interiors, as in a conventional material, but strictly from the GBs and GBJs. Last, is the τ_{CRSS} anisotropy, in which the critical stresses to activate the b-parallel slip planes are easier than the b-inclined slip planes. Together these factors can lead to a dependence of the number and type of slip systems activated on the direction of loading and hence plastic anisotropy.

3. Model characterization

To examine plastic anisotropy, the material is deformed in compression in one of two orthogonal directions, either along the growth direction, that is, normal to the twin boundaries (z-direction in Figure 1), or parallel to the twin boundaries (x-direction). Adopting the nomenclature of experimental studies [16] to which we will compare our results, the former test is called the 90° test and the latter the 0° test. In the 0° test, a strain rate of 0.001 s^{-1} is applied along the x-axis while the boundary conditions in the other two directions are set stress-free, ensuring simple compression boundary conditions. Likewise, in the 90° test, the same rate is applied in the z-direction and the other two directions are stress-free.

¹ We limit the total number of such simultaneous slip events; however, find that it rarely exceeds eight in the calculations that follow.

As part of the material set up, two material parameters, associated with the plastic part of the constitutive model, namely equation (3), require characterization: the reference shear strain rate $\dot{\gamma}_0$ and the rate sensitivity m . For this purpose, we use two stress-strain curves taken from the 0° and 90° compression tests made on NT Cu at room temperature by You et al. [16]. The NT Cu had an average grain size $D = 3000$ nm and twin thickness $\lambda = 30$ nm, which we also assign to our NT model. These experimental tests were conducted at a strain rate of 0.001 s^{-1} and therefore in the model, we set $\dot{\gamma}_0 = 0.001 \text{ s}^{-1}$. We set m equal to 0.1, which is a common value for face centered cubic (fcc) NC metals [50], like the Cu we model here.

Figure 6 compares the measurement with the model result for $D = 3000$ nm and $\lambda = 30$ nm and the initial texture in Figure 2. With this set of values for $\dot{\gamma}_0$ and m , the model is able to capture the pronounced anisotropy between the two curves, the fact that the 90° test is the stronger of the two, and the variation in flow stress with strain. Slight changes in m , ± 0.02 , provide similar agreement. In all calculations that follow, these parameters remained fixed.

4. Results and discussion

4.1 Effect of the grain size, D

In the actual NT material, the grain size D varies within the material. However D is typically much larger than the twin spacing $D \gg \lambda$ and hence it would be expected that size effects in D would be weak relative to those in λ . To gain some insight into the effect of D , we performed calculations for $D = 500$ nm, and 1500 nm with $\lambda = 30$ nm, maintaining that $D \gg \lambda$, and include the results in Figure 6 with $D = 3000$ nm. As shown, the strength increases as D decreases, which is to be anticipated. More importantly, the D -effect is weak provided $D \gg \lambda$, and hence we will focus the calculations to follow on size effects in λ .

4.2 Effect of initial texture

NT materials possess sharp textures, which can be expected to be partly responsible for the plastic anisotropy seen experimentally. To reveal the effect of texture, we repeated the calculation for NT material with $\lambda = 30$ nm, $D = 3000$ nm (in Fig. 6) but either with no starting texture (random) or an ideal (111) starting texture (Figure 7(a)). For the random texture, the NT boundary plane normals are randomly oriented with respect to the sample, whereas for the ideal

(111) texture, they are all perfectly aligned with the z-axis. In both cases, the crystallographic orientations remain random in plane.

Figure 8 compares the 0° and 90° flow stress curves for these extreme cases with those predicted when the experimental texture is used as input. Without an initial texture (i.e., random texture), the plastic anisotropy is negligible. This result is consistent with reports on equiaxial-grained NT Cu, which exhibits near plastic isotropy because of the randomly oriented twin layers [17]. In contrast, with an ideal (111) initial texture, the plastic anisotropy is significant, with the 90° test being the stronger of the two, as with the experimental (“natural”) (111) initial texture (Figure 8). Altogether these results show that texture causes the 90° test to have the stronger flow stress than the 0° test. Further, we observe that a seemingly small change in the initial texture from the natural (111) initial texture to the ideal (111) one can lead to a few significant changes in flow stress-strain behavior. First, the material strengthens in both the 0° and 90° loading directions. Second, initial-texture sharpening has a greater impact on the 90° test compared to the 0° test. In other words, the plastic anisotropy increases with texture sharpening largely because the 90° test is much more sensitive to texture than the 0° test.

When texture dominates, the flow stress would be expected to be roughly proportional to the Taylor factor (TS) associated with each test. Here, we calculate the Taylor factor for each twin lamella as the inverse of the average of the five largest Schmid factors among its b-inclined slip systems and then for the entire NT material, compute TS as the average value from all twin lamellae. In efforts to correlate this measure with anisotropy between the 90° and 0° tests, we consider $\Delta TS = (TS_{90^\circ} - TS_{0^\circ})$, where TS_{90° and TS_{0° are the Taylor factors for 90° and 0° compression tests, respectively. For the random texture, ΔTS is zero. For the ideal (111) texture it is ~ 0.68 , which is twice ΔTS for natural (111) texture (~ 0.35). This increase in ΔTS is largely due to the increase in TS_{90° . When the texture sharpens from the natural (111) texture to the ideal one, TS_{90° increases from 3.33 to 3.67, whereas TS_{0° only increases from 2.98 to 2.99. Taken together, we find that this simple geometric TS measure explains 1) the loss of anisotropy for an initial random texture, 2) the pronounced increase in anisotropy when changing the initial texture from the natural to the ideal one, and 3) the higher sensitivity of the 90° test to the initial texture change.

One of the useful predictions of CP mechanics based codes pertains to the slip system activity underlying the deformation. How much one type of slip contributes to the deformation relative to another depends on both the 1) loading direction with respect to the texture (geometry) and 2) difference in their τ_{CRSS} values (material). The orientation relationship between both 0° and 90° loading directions with respect to the natural (111) texture is such that the Schmid factors on the b-inclined planes will tend to be larger than on the b-parallel planes than b-inclined planes. Thus, geometric considerations alone would expect that deformation in both 0° and 90° loading test directions will engage more b-inclined slip than b-parallel slip, since the latter is geometrically harder. Further, in the natural (111) texture, the crystals are randomly oriented within the x - y plane but well aligned in the z -direction within a 25° deviation. Consequently, in the 90° compression test few grains are well oriented for parallel slip but all grains are oriented for inclined slip; whereas in the 0° compression test most grains are oriented for both parallel and inclined slip. Thus, the 0° compression test direction is more suitably oriented than the 90° compression test direction to activate the b-parallel slip within the twin lamellae. However, while the b-parallel systems are the geometrically harder slip mode in the 0° and 90° tests, they are at the same time the “physically easier” to activate. The characteristic length scale for activating b-inclined slip is λ , which is much smaller than the characteristic length scale D for activating b-parallel slip, and hence the activation stresses for b-inclined slip are much greater. Thus, it is not obvious *a priori*, which slip type would predominate in a given test and for a given NT λ .

To examine the strain evolution of slip activity from simulation, the relative activity (RA_m) of a given slip mode m , and the number of slip events of each mode (N_m) within each twin lamella and a given strain increment are calculated. RA_m is given by [51]:

$$RA_m = \frac{\dot{\Gamma}_m}{\sum_{m=1}^{N_m} \dot{\Gamma}_m}; \quad (5)$$

where N_m is the total number of slip modes, which for NT Cu, is two: inclined slip and parallel slip. In Eq. (5), $\dot{\Gamma}_m$ is the total slip rate of mode m in all twin lamellae,

$$\dot{\Gamma}_m = \sum_{g=1}^{N_g} \dot{\Gamma}_m^g \quad (6)$$

where N_g is the total number of twin lamellae, and $\dot{\Gamma}_m^g$ is the total slip rate of mode m in twin lamella g , which is defined as,

$$\dot{\Gamma}_m^g = \sum_{s=1}^{N_s^m} \dot{\gamma}_{s,m}^g \quad (7)$$

where $\dot{\gamma}_{s,m}^g$ is the slip rate of system s in mode m of twin element g , calculated via Eq. (3).

Figure 9 shows the strain evolution of RA_m of the b-parallel and b-inclined slip systems in the 0° and 90° tests when starting with the natural (111) texture. Due to the discrete and inhomogeneous nature of slip among the twin lamellae, RA_m experiences fluctuations from one strain step to another. In the initial part of plastic deformation, b-parallel slip dominates for both 90° and 0° compression tests. During this first straining period, those grains that are oriented to deform by the easier b-parallel slip accommodate nearly all the deformation. At this point, although inclined slip is geometrically possible in all grains, the macroscopic stress is not sufficiently high to activate the harder inclined slip systems. However as strain levels increase beyond 0.05, the relative contribution of b-inclined slip increases rapidly. Eventually a steady state is reached where both 0° and 90° tests activate more b-inclined slip than b-parallel slip. However, they do not activate similar fractions of the harder b-inclined slip system. The 90° test activates 55% of b-inclined slip ($\sim 45\%$ b-parallel slip), whereas the 0° test activates 65% of b-inclined slip ($\sim 35\%$ b-parallel slip).

From the above, we find that there is a transition from b-parallel slip to b-inclined slip as straining. It may be argued that the change may be a result of texture evolution. To see whether this is the case, Figure 7(b) and (c) compares the deformation textures at 6% strain when starting with the natural (111), ideal (111), and random textures. The final texture after 6% strain is similar between the 0° and 90° tests. The pronounced anisotropy seen within the moderately small straining periods of 6% is, therefore, not due to differences in texture evolution between the two test directions. Since the texture does not evolve in the small strain period tested, the transition from less b-parallel slip to more b-inclined slip results from the increase in stress enabling more grains to activate more b-inclined slip.

On this basis, a difference slip pattern can be expected when starting with the ideal (111) texture, since no grains are initially oriented for b-parallel slip. Figure 9 shows the relative slip activities for the NT material with the ideal (111) initial texture. For the 0° test, the relative activities between b-parallel slip and b-inclined slip have not changed significantly from that of the natural (111) texture, eventually achieving a steady state with more b-inclined slip (75%) contribution and hence less b-parallel slip (25%). This comparatively small change can be expected since the texture relative to the 0° test direction remains random in the x-y plane. For

the 90° test, however, the relative activities of b-parallel and b-inclined slip have switched. The difference is particularly noticeable for strains up to 3%, where b-inclined slip dominates, which can be expected since in the starting ideal (111) texture, no grains are initially oriented for a non-zero RSS on the b-parallel slip systems. After 3% strain, the contribution of b-parallel slip increases rapidly, and concomitantly, that of b-inclined slip reduces. The increase in b-parallel slip activity is caused by slip-induced lattice rotations. As the τ_{CRSS} values for b-parallel slip are 20 ~ 30 times smaller than that for b-inclined slip, even a small lattice rotation, not detectable in a bulk texture, can cause the resolved shear stress to become non-zero promoting b-parallel slip. Thus, the steady-state slip pattern in the 90° test has reversed, involving much more b-parallel slip than b-inclined slip when sharpening the texture from the natural (111) one to the ideal (111) one.

The analyses of the geometric Taylor factor and relative activities of b-parallel and b-inclined slip together suggest that the larger flow stress in the 90° test and increased plastic anisotropy seen when changing from a (111) natural to ideal (111) initial texture is primarily a consequence of texture. Specifically, texture strengthening of the texture causes the 90° test to utilize an even higher fraction of the harder b-inclined slip systems compared to the weaker, natural (111) texture.

4.3 Strength scaling with twin thickness λ

Next we use the model to explore the size effects in λ on strength, strain hardening, and plastic anisotropy. In Figures 11(a) and (b) the variation in the calculated yield stresses for $D = 3000$ nm with twin layer thicknesses in the range of $\lambda > 10$ nm are shown for the 90° and 0° tests. For validation, results for the 90° and 0° strength of NT Cu samples found in the literature are also included [6, 14, 16, 52-54]. In these experimental studies, the degree of texture sharpness would have been hard to specify, so to span a range of possible initial textures, we have included in Figure 10 calculations for a random texture, the experimental (natural) texture by You et al. [16], and the ideal (111) texture. Because we found D to have a little effect (as long as $\lambda \ll D$), a similar strength scaling in D is not considered. However, D likely varied among these NT Cu samples and so we included results for $\lambda = 30$ nm spanning $D = 500$ nm - 3000 nm (indicated by error bars). Overall, the model appears to achieve reasonable agreement within the range of

measurements, even in spite of its idealized NT microstructure and assumptions on GB-driven dislocation emission.

The number of experimental data points is too few to dependably indicate a size scaling in λ . The model, on the other hand, suggests that yield strength scales inversely with λ . Interestingly, the calculated strengths in Figure 10 do not follow a Hall-Petch scaling as seen in some NC metals and layered composites [55] or a $\log(\lambda)/\lambda$ scaling characteristic of some nanolayered metals [56]. Furthermore, for the 90° strengths, this size effect in λ is seen to intensify as the texture sharpens; that is, NT materials with a more highly oriented (111) texture would strengthen faster with decreasing λ . Regarding the nature of the size effect, it is worth mentioning that the present model predicted a Hall-Petch scaling in grain size for NC Ni, which was modeled as an aggregate of equiaxed grains, in excellent agreement with a conglomeration of experimental data sets [31]. From this, it could be speculated that architecture of the nanostructure (i.e., equiaxed crystals vs. thin lamellae) plays a role in the strength scaling in microstructural size due to its effects on the strength to nucleate and propagate dislocations.

Using the same model, we examine the effect of λ on the flow stress curve, paying particular attention to strain hardening. Figure 11 shows the calculated stress-strain curves for $\lambda = 20$ nm, 30 nm, 50 nm, and 100 nm. Overall, as λ increases, the material weakens but the strain hardening increases. The stress-strain curves for $\lambda = 30$ nm, which correspond well to those measured by You et al. [16], and $\lambda = 20$ nm exhibit negligible strain hardening, whereas those for $\lambda = 100$ nm show noticeable strain hardening.

Strain hardening in this material model does not arise from dislocation accumulation as in coarse-grained metals, since the model assumes all emitted dislocations are fully absorbed at grain boundaries and hence are not stored inside the grains. The strain hardening could, however, arise from statistical variation in dislocation emission, since for each increment in strain, there is a finite chance that the critical stress to emit the next dislocation could be higher. As we have modeled it, the longer and ‘weaker’ sources in the boundary are just as likely to be available as the shorter and ‘harder’ sources. To test this idea, we carried out additional calculations with the statistical variation in τ_{CRSS} in time and space removed. We assigned at the outset all sources for b-inclined slip the same τ_{CRSS} corresponding to the mean value for the λ of interest and likewise, all sources for b-parallel slip the same τ_{CRSS} associated with the mean value for the D of interest.

Throughout the straining, the value given is held constant, as if the activation stress for dislocation emission at that boundary had reached steady state. Figure 11 includes the stress-strain curves resulting from this constant τ_{CRSS} calculation. As shown, using a constant τ_{CRSS} has suppressed strain hardening for all λ . The comparison shows that temporal and spatial statistical activation of dislocations from grain boundaries can lead to strain hardening. This finding implies that greater dispersions in τ_{CRSS} lead to more strain hardening. In the present model, this effect would imply a size effect in strain hardening since the coefficient of variation in τ_{CRSS} decreases as λ decreases (See Table 1). It explains why we observe reduced strain hardening with decreasing λ in Fig. 11, which has already been confirmed by recent experiments on the tensile behavior of columnar grained NT Cu [14].

4.4 Twin thickness dependent plastic anisotropy

We last explore the effect of λ on plastic anisotropy. As we have shown earlier, plastic anisotropy arises predominantly as a result of the initial texture. Further, it is anticipated that as NT materials are made with finer λ , their initial texture would not change significantly, and the strong (111) in-plane isotropic texture, which we call the natural (111) texture, would apply for all λ . Figure 12 shows the differences in the calculated 0.2% yield stress between the 90° and 0° tests, denoted as $\psi = \sigma_{90} - \sigma_0$, when starting with the natural (111) texture and $D = 3000$ nm. For all λ , the 90° flow stress remains the stronger of the two test directions. This consistency in the order of anisotropy is expected since in all these cases, the initial texture is the same. However, we noticed that $\psi = \sigma_{90} - \sigma_0$, increases with decreases in λ . Evidently, the calculations are indicating a possible additional size effect on the plastic anisotropy, wherein finer λ leads to greater anisotropy in the stress-strain response.

This additional size effect could arise if reducing λ caused a change in the relative slip activities of b-parallel and b-inclined slip. As before, we calculate the variation in RA_m (equation 5) with strain and find that it evolves in the same manner for all λ from 15 nm to 100 nm as it does for $\lambda = 30$ nm in Figure 10, achieving a steady-state value after 0.5% strain. Figure 13 presents this steady-state value as a function of λ , demonstrating that RA_m is unaffected by a refinement in λ . Thus, stronger plastic anisotropy with decreasing λ is not a consequence of transitions in the relative activities of b-parallel and b-inclined slip.

With the same natural (111) initial texture and contribution of b-inclined slip unchanged for all λ , the main dependency on λ remaining lies in the distribution of τ_{CRSS} for b-inclined slip (See Figure 4 and Table 1). As λ decreases, the mean CRSS increases and coefficient of variation in τ_{CRSS} decreases. For comparison, the mean τ_{CRSS} value is also plotted on Figure 12. As shown, the yield stress anisotropy ψ and the mean τ_{CRSS} increase in a similar manner with λ . The similarity suggests that, to first order, the ratio of ψ to mean τ_{CRSS} would be constant. For all λ , it ranges from 0.54 to 0.63, which could be considered a small variation in light of the spatial and temporal statistical variation in τ_{CRSS} involved in determining the strength of NT Cu calculated here. Thus, through an increase in the CRSS to emit dislocations, reducing λ enhances the plastic anisotropy of NT Cu even when the initial texture is the same.

5. Conclusions

In this work, we develop a crystal plasticity finite element model for nanotwinned (NT) materials that takes into account for the effect of the strong initial texture, texture evolution, and grain-grain and twin-twin interactions during deformation. Unlike in conventional crystal plasticity models, in this model, plasticity occurs by discrete slip events from grain boundary to grain boundary. Dislocations emanate exclusively from internal boundaries and dislocation source lengths are limited by the twin thickness λ , and dislocation slip distances are limited by the grain size D . We use the model to examine texture effects and size effects in λ and D on material strength, strain hardening, and plastic anisotropy by computing the deformation response for 0° and 90° tests for different λ ranging from 15 nm to 100 nm and D from 500 nm to 3000 nm.

- a) Experimental studies have reported that the manufacturing of nanotwinned Cu can result in equiaxial-grained NT Cu with a random texture and no plastic anisotropy or in columnar NT Cu with a strong (111) in-plane isotropic texture and pronounced plastic anisotropy. Despite many sources of anisotropy and the discrete nature of slip captured in the model, the model suggests that the plastic anisotropy seen experimentally in columnar NT Cu can be attributed predominantly to texture. Plastic anisotropy was suppressed in the equiaxial-grained NT Cu material but strong in the columnar NT in very good agreement with experimental observations. Sharpening of the (111) texture to a higher alignment of the (111) poles through-the-thickness of the foil serves to strengthen the plastic anisotropy by strengthening

proportionally more the flow stress in the 90° test (applied normal to the nanotwinned boundaries) than the 0° test (applied in-plane). The analysis reveals that this strengthening results from activating more slip events inclined non-planar to the twin boundaries in more twin lamellae.

- b) We find that the flow stress decreases as λ increases in a manner that is in good agreement with experimental data from a large number of studies. These calculations involved different grain sizes D values ranging from 500 nm to 3000 nm and for this range, where $D \gg \lambda$, we find that D has a relatively insignificant effect on the flow stress.
- c) Strain hardening in the stress-strain curves is predicted to increase as λ increases, despite the ideal condition of no dislocation storage within the lamellae. Analysis of the model results finds that spatial- and time-varying changes in the τ_{CRSS} to emit dislocations from grain boundaries leads to straining hardening, with more dispersion in τ_{CRSS} leading to higher strain hardening. In the ideal case that dislocations are emitted from the grain boundary with a constant, non-varying activation stress, strain hardening is removed.
- d) The analysis indicates that for the same strong (111) in-plane isotropic texture, the plastic anisotropy in yield stress ought to increase with reduction in twin thickness as a consequence of the concomitant increase in the stress to emit dislocations.

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Figure 1 (a) Schematic of a NT Cu sample with columnar grains. (b) Plane view of the NT Cu sample. The compression perpendicular to the columnar axis is defined as 90° compression. (c) A portion of a single columnar grain including twin/matrix structure.

Figure 2 $\{111\}$, $\{110\}$ and $\{112\}$ pole figures of the initial texture of the columnar-grained NT Cu. This texture is used to initialize the model microstructure prior to application of the load and is referred to as the ‘natural (111) texture’ in the text.

Figure 3 (a) Schematic of a twin lamella in one grain with a dislocation nucleating from a GB on an inclined slip plane (left) and from a grain boundary junction (GBJ) on a parallel slip plane (right). (b) Planar views of the inclined slip plane (left) and the parallel slip plane (right).

Figure 4 Probability density distributions for τ_{CRSS} for activating dislocation sources from GBs for different twin lamella thickness λ .

Figure 5 Probability density distributions for τ_{CRSS} for activating dislocation sources from GBJs for different grain sizes D .

Figure 6 Comparison of experimental [16] and calculated stress-strain curves for columnar-grained NT Cu with twin thickness $\lambda = 30$ nm and different grain sizes D .

Figure 7 (111) pole figures of the (a) initial textures; and calculated deformation textures at 6% strain under (b) 90° compression; (c) 0° compression. (Left: natural (111) texture. Middle: ideal (111) texture. Right: random texture. Legend is in units of m.r.d. (multiple of random distribution)).

Figure 8 Comparison of calculated stress-strain curves for natural (111) texture, ideal (111) texture and random texture with $\lambda = 30$ nm and $D = 3000$ nm. (Solid lines: 90° compression. Dashed lines: 0° compression.)

Figure 9 Relative activities (RA) of the b-inclined and b-parallel planes for natural and ideal (111) textures with $\lambda = 30$ nm (a) under 90° compression, (b) under 0° compression.

Figure 10 Comparison of experimental and calculated yield strengths for columnar-grained NT Cu (a) under 90° compression, (b) under 0° compression. The error bars on the calculated strengths for $\lambda = 30$ nm cover results for $D = 500$ nm to 3000 nm. Experimental data were obtained by nanoindentation marked with an “I”, compression marked with a “C” for tension marked with a “T”. (In nanoindentation tests, the yield strength was approximated as hardness divided by 3.0 [14].)

Figure 11 Stress-strain curves employing either constant τ_{CRSS} and statistical τ_{CRSS} values for various twin layer thicknesses λ : (a) 90° compression; (b) 0° compression.

Figure 12 Comparison of the variation in plastic anisotropy, $\psi = \sigma_{90} - \sigma_0$, with twin thickness λ for natural (111) texture with the mean τ_{CRSS} for b-inclined slip.

Figure 13 Steady-state value of RA (the average value of RA from 1% to 5% strain) for b-inclined and b-parallel slip as a function of λ from 15 nm to 100 nm.

Table 1 List of parameters of the τ_{CRSS} distributions for emitting dislocations

Twin layer thickness (nm)	Median (MPa)	Mean (MPa)	Standard deviation (MPa)	Coefficient of variation
10	234.5898	234.3374	1.3628	5.8157E-3
15	229.2909	226.7398	8.2717	0.0365
20	222.0146	218.6064	14.5610	0.0666
30	206.2007	202.5845	24.8259	0.1225
40	191.2998	189.6319	31.5755	0.1665
50	178.0782	178.1723	36.5982	0.2054
75	151.8078	156.4649	43.9794	0.2811
100	131.5614	140.8191	47.7140	0.3388
Grain size (nm)				
500	33.2429	39.5977	20.9013	0.5278
1500	13.8295	17.0287	11.2570	0.6611
3000	7.7823	9.7254	7.1654	0.7368

Statistical dislocation activation from grain boundaries and its role in the plastic anisotropy of nanotwinned copper

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Graphical abstract