Predicting the size scaling in strength of nanolayered materials by a discrete slip crystal plasticity model

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Abstract

The main attraction of metallic nanolayered composites (MNCs) lies not only with their five- to ten-fold increases in strength over that of their constituents, but also in the tunability of their superior strength with nanolayer thickness. While the size scaling in strength prevails in many MNC material systems, the size scaling cannot be accurately predicted with crystal plasticity framework. Here, we present a crystal plasticity based computational method that considers plasticity to occur in grain boundary-controlled discrete slip events and apply it to predict the deformation response and underlying mechanisms in Cu/Nb MNCs. Predicted tensile stress-strain responses are shown to achieve agreement with measurements for four distinct nanolayer thicknesses, without introducing adjustable parameters. The model predicts the Hall-Petch size scaling of strength on layer thickness and the rising plastic anisotropy as the layer thickness reduces. Analysis of the results indicates that the origin of the layer size effect on strength results from the limits layer thickness places on the lengths of dislocations sources lying in the grain boundaries.

Keywords: Crystal plasticity, Dislocations, Grain boundaries, Layered material, Finite elements

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1. Introduction

With the progress in new nanotechnologies, metallic nanolayered composites (MNCs) made from constituents with different physical properties have been drawing ever-increasing attention. They have demonstrated ultra-high strength compared to bulk constituents (Clemens et al., 1999; Misra et al., 2005), high radiation damage tolerance (Zhang et al., 2007), shock resistance (Han et al., 2011), and thermal stability (Zheng et al., 2013). In particular, strengths of MNCs range from three to ten times that of coarse-layered counterparts (layer thickness $h \sim 10^{-3}$ -10^{-5} m). Impressive enhancements have been qualitatively attributed to the fine layers of nanoscale dimension ($h \sim 10$ - 50 nm). Based on observations from numerous studies, it has become well known that the strengths of traditional polycrystalline metals scale inversely with the finest microstructural length scale (e.g., grain size) (Armstrong, 2013, 2014; Armstrong, 2016; Beyerlein et al., 2012; Beyerlein et al., 2014b; Mara and Beyerlein, 2014). It can, therefore, be expected that three- to ten-fold increases in strength would arise when the layer thickness h is reduced to nanoscale dimensions, often by three to five orders of magnitude from the coarse layer thicknesses. Besides the layer thickness, there are other factors strongly affecting the strength of MNCs, such as crystallographic orientation (Beyerlein et al., 2014a, Beyerlein et al., 2014b), the arrangement of interfaces and constituent shapes (Buehler and Misra, 2019; Demkowicz, 2019).

The other desirable properties that MNCs exhibit, in addition to strength, has inspired intense study to identify and understand the underlying deformation mechanisms and origins of the size scaling of h on strength. Many works have proposed that the form of the size scaling depends on how internal grain boundaries and biphase interfaces interact with the moving dislocations. In coarse-layered composites, an individual layer contains many smaller grains and

the size scaling in strength would depend on the intralayer grain size (Khadyko et al., 2016; Lyu et al., 2017; Ruppert et al., 2016). In the finer MNCs of interest here (h < 500 nm), a single grain spans the layers, and hence the biphase interfaces confine dislocation motion in the grain. In this case, Misra et al. (Misra et al., 2005) proposed three mechanistic regimes in MNCs as a function of individual layer thickness h: i) In the Hall–Petch (dislocation pile-up) regime (h >100 nm), the strength mechanism is analogous to the grain-boundary strengthening mechanism, in which mobile dislocations are blocked at the interface and form pile-ups. The strength is expected to scale as $h^{-1/2}$. ii) In confined layer slip, (CLS) regime (h < 100nm), a dislocation threads within the layer with the dislocation propagation stress scaling as $\ln(h)/h$ (Anderson et al., 1999). iii) In the interface-crossing regime (h < 10 nm), dislocation transmission across interfaces controls strength. In this regime, the strength is determined by the stress to transmit a dislocation and hence is not dependent on layer thickness. This can manifest as a saturation in the strength (or hardness) (Kalkman et al., 2002; Niu et al., 2012). Direct observation of CLS has been reported in Cu/Nb nanolayers (Li et al., 2012b; Liu et al., 2018), but otherwise such in-situ experiments can be challenging. Many studies, instead, use strength tests, such as in-plane tension, nanopillar compression, or nanoindentation hardness, on MNCs made with different h to match size scalings in strengths to one of the three regimes (i)-(iii) to indirectly discern the governing mechanism. A recent assessment of numerous reports demonstrated, however, that measured h-scaling in strength for all systems could be fit to either $h^{-1/2}$ or $\ln(h)/h$, indicating that such an inverse approach for identifying mechanisms may not be conclusive (Subedi et al., 2018).

Thus far, most computational efforts to identify the key mechanisms have involved atomistic modeling of the deformation behavior of Cu/Nb MNCs, especially for single crystalline Cu/Nb. Collectively, the simulations implied that interfaces play a critical role in the

deformation of Cu/Nb MNCs by acting as sources for dislocation nucleation and barriers to dislocation slip transmission (Wang et al., 2008; Wang et al., 2009). In NC MNCs, dislocation sources lie in the grain boundaries and interfaces. Layer thickness does not affect the stress to activate interface sources but it affects the stress to activate grain boundary sources (Chen et al., 2018; Zhang et al., 2016). Recently, atomic-scale simulations were employed to investigate microstructural size scaling in the strength of nanocrystalline (NC) Cu/Nb MNCs under an applied uniaxial tension (Huang et al., 2017). It was found that plasticity initiates by emission of dislocations from the junctions within both phases, where grain boundaries and interfaces meet, rather than at the biphase interfaces. Further, we mention that other MD and experimental works focus on nanoindentation (Clemens et al., 1999; Misra et al., 2005), which applies a high local stress concentration that can promote dislocation nucleation from all possible interface and grain boundary sources.

Despite the insights gained by in-situ scanning electron microscopy (SEM) (Li et al., 2012a) and atomistic simulations (Abdolrahim et al., 2014; Huang et al., 2017), the origin of the size effects for different tests, loading directions, and starting textures and microstructures, is not well understood. The time and length scales of the atomistic simulations prevent them from examining the combined effects of texture evolution and dislocation activity in a rate and temperature regime consistent with laboratory test conditions.

For many decades, crystal plasticity finite element (CPFE) models have served as powerful models for relating polycrystalline texture evolution and subgrain dislocation and twinning activity with macroscopic stress-strain response (Bronkhorst et al., 2006; Bronkhorst et al., 1992; Kalidindi et al., 1992; Knezevic and Beyerlein, 2018; R. Kalidindi, 2001; Roters et al., 2010). However, most CPFE models assume slip occurs homogeneously at a material point, an

assumption that is suitable for the plastic deformation of coarse-grained materials. Standard CPFE models also adopt phenomenological hardening laws for slip that presume *a priori* the type of hardening response or grain size effects on hardening, as well as introducing a number of parameters (Ardeljan et al., 2015; Beyerlein and Tomé, 2007; Hansen et al., 2013; Knezevic et al., 2014; Mayeur et al., 2015; Mayeur et al., 2013). For nanostructured metals, however, the nanoscale dimensions of the crystals are similar to that of the individual dislocation (a few nm) and the assumption of homogeneous plasticity breaks down.

In an attempt to overcome these constraints, Yuan et al. (Yuan et al., 2015) recently developed a discrete slip (DS) model for nanocrystalline (NC) metals in which plasticity occurs by discrete slip events activated statistically from grain boundaries. The basic idea is that the grain size physically limits the segment lengths of GB dislocation sources, giving rise to a grain size effect in the stress to activate these sources, and also limits the amount of shear strain a dislocation gliding across the grain can accommodate. The DS model was incorporated into a 3D CPFE microstructural model of a NC FCC material (either Ni or Cu) in order to link plasticity occurring via discrete slip events to the crystallographic grain orientation, and applied stress (Yuan et al., 2015; Yuan et al., 2016). The DS-CPFE model predicted the emergence of Hall-Petch grain size scaling of yield strength and peak strengths, in agreement with several experimental NC Ni and Cu studies (Ebrahimi et al., 1999; Schuh et al., 2003).

In this work, we present a discrete slip crystal plasticity framework to study the plastic deformation in an MNC. We apply it to examine the origins of size effects on strength in a two-phase Cu/Nb nanolayered composites. This model relates nanocrystal size and texture to the anisotropic flow response of nanolayered composites and quantifies the relationships between the layer thickness h and plastic anisotropy in Cu/Nb nanolayered composites. It uses, as input,

measurable quantities and introduces no adjustable parameters. We demonstrate that the calculations achieve agreement with the experimentally seen scaling between yield strength and layer thickness, flow response, and plastic anisotropy. Analysis of the underlying slip activity indicates that the origin of the layer size effect results from the limits layer thickness places on the lengths of dislocations sources lying in the grain boundaries and interfaces. We show that stochastic evolution of source strengths in GBs gives rise to strain hardening. Notably the model predicts Hall-Petch scaling in yield strength and increasing plastic anisotropy with reductions in layer thickness in agreement with tensile tests on bulk Cu/Nb nanolaminates. We show that the latter is a consequence of the TD and RD flow stresses adopting individual size scalings in strength.

2. Methodology

2.1 Basic CPFE framework

The CPFE framework and constitutive law we use here is standard, and thus, it is described in brief below, while the discrete-slip, plasticity model is presented shortly in full. The constitutive formulation is written as a user-defined material (UMAT) subroutine developed by Marin (Marin and Dawson, 1998) and implemented into the finite element software Abaqus CAE. The kinematics of crystal deformation is based on the multiplicative decomposition of the deformation gradient $\boldsymbol{F}$:

$$F = F^e F^p \tag{1}$$

where F_e is the elastic gradient, and F_p is the plastic gradient. The evolution of the plastic component is also defined as:

$$\dot{F}^p = L^p F^p \tag{2}$$

where L^P is the velocity gradient, which accounts for the plastic deformation generated by the dislocation slip and can be calculated by the summation of the plastic flow of all slip systems:

$$L^P = \sum_{\alpha=1}^{N} \dot{\gamma^\alpha}\, \boldsymbol{b}^\alpha \otimes \boldsymbol{n}^\alpha \tag{3}$$

where $\boldsymbol{b}^\alpha$ and $\boldsymbol{n}^\alpha$ are the slip direction and slip plane normal for the slip system α, $\dot{\gamma^\alpha}$ is the shear strain rate on slip system α, and N is the number of slip systems.

2.2 The discrete slip model in nanocrystalline grains

Here, building upon the previous discrete slip crystal plasticity model for single-phase NC materials (Yuan et al., 2015), we present a geometrically based, statistical dislocation emission model for driving discrete slip events in a two-phase MNC system. We first describe the underlying mechanisms and corresponding mechanics formulation. We then follow with the specific application to grain boundaries lying with the NC layers of an MNC.

In this model, the nanograins are assumed to be free of dislocations and the grain boundaries (GBs) to be defective and serving as the sole sources and sinks for dislocations in the material. When acted upon by an appropriately high stress, prevailing locally in a volume around the source, a dislocation or dislocations can protrude out from the GBs from the source, and glide on the {111} planes within the nanograin until it intersects with the other portion of the surrounding GBs. Idealized here as perfect sinks, the grain boundaries absorb the impinging dislocation from the grain. Hence, after the slip event, the grain interior remains free of defects, and the GBs, once again, full of defects.

In this situation, the stress needed for plastic deformation in this grain corresponds to the stress to emit a gliding dislocation from a GB source. We refer to this critical stress as the critical resolved shear stress (τ_{CRSS}) and the amount of glide incurred from one slip event by one dislocation as $\gamma_{discrete}$. The former is a scalar value, and is to be compared with the resolved shear stress on the slip system, defined as the projection of the stress tensor in the plane of the dislocation and along the slip direction. The τ_{CRSS} is a widely used term for dislocation glide resistance, but how it is formulated in CPFE models depends on the physical obstacle that opposes glide.

In this model, the aforementioned discrete dislocation slip event is pictured to take place in three sequential steps: formation of sources in the GBs, emission of dislocations into the grain from the source, and propagation of the dislocation after emission. Each requires a separate critical stress. The τ_{CRSS} representing a successful slip event is determined by the largest step of the three, the one that prevail for the ambient deformation conditions of interest here. In the case in which grain boundaries contain pre-existing defects and the grain interiors are dislocation-free, the τ_{CRSS} is governed by the stress to first emanate the dislocation from the GB source, the second step described above. This assumption is consistent with the finding from atomistic simulations that the activation barrier for dislocation propagation is larger than that for dislocation nucleation (Bitzek et al., 2008).

The GB dislocation sources are idealized as the double-pinned dislocation segment with the length, L, as shown in Figure 1. Emitting the dislocation from this L-source corresponds to the critical stress needed to expand the source segment into the nanograin on a {111} glide plane to an unstable configuration, at which point the dislocation can "breakaway" and glide fully across the grain without additional increments in stress. Reaching the unstable configuration

requires the source length L to extend and bow out. The dislocation line tension resists this motion. Following closely this emission mechanism is Foreman's formula (Foreman, 1967), which is adopted here for the critical resolved shear stress τ_{CRSS}. Accordingly, the τ_{CRSS} required to overcome the line tension generated in expanding a dislocation from a segment of length L in the GB is,

$$\tau_{CRSS} = \frac{A}{2\pi}\frac{\mu b}{L}\log\left(\frac{L}{r_0}\right) \tag{4}$$

where A is a pre-factor on the order of unity, μ is the shear modulus, b is the magnitude of the Burgers vector, r_0 is the dislocation core radius, and L is the dislocation source length. The τ_{CRSS} is controlled by the source length L. The shorter L is, the larger the stress needed for propagation.

Each time a dislocation emanates and glides across a nanograin, the nanograin is strained by a discrete amount of shear $\gamma_{discrete}$. The shear displacement is given by b, the value of the dislocation Burgers vector, an intrinsic material value, while the distance over which this displacement occurs depends on the orientation of the slip plane on which the dislocation glides with respect to the grain boundaries and the distance between adjacent boundaries. In a Cartesian based global coordinate system, x, y, z, the grain dimensions can be characterized by its lengths L_x, L_y, and L_z, along these three axes, respectively. For a dislocation gliding on a plane with normal n, $\gamma_{discrete}$ can be calculated by:

$$\gamma_{discrete} = \gamma_x cos^2\theta_x + \gamma_y cos^2\theta_y + \gamma_z cos^2\theta_z \tag{5}$$

where $\gamma_x = \frac{bsin\beta_x}{L_x}$, $\gamma_y = \frac{bsin\beta_y}{L_y}$, $\gamma_z = \frac{bsin\beta_z}{L_z}$ are the shear strains projected in three orthogonal axis directions, θ is the angle between the normal of the slip plane n and the corresponding axis,

and β is the angle between the Burgers vector and the corresponding axis. The slip plane angles are constrained by $cos^2\theta_x + cos^2\theta_y + cos^2\theta_z = 1$.

The Burgers vector b and slip plane n combination refers to an independent slip system. Depending on the crystal and the material, there are usually more than one slip mode, consisting of many crystallographically equivalent but independently oriented slip systems. Accordingly, at this point, we mention that the τ_{CRSS} and $\gamma_{discrete}$ depend on the slip system α, and hence we denote them using a superscript α hereinafter as τ^{α}_{CRSS} and $\gamma^{\alpha}_{discrete}$.

The shear strain rate corresponding to the glide of a dislocation activated on slip system α is calculated using a flow rule, for which we adopt the conventional visco-plastic, rate-dependent power law form:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left[\frac{|\tau^{\alpha}|}{\tau^{\alpha}_{CRSS}}\right]^{\frac{1}{m}} sign(\tau^{\alpha}) \tag{6}$$

where $\dot{\gamma}_0$ is a reference shear strain rate, τ^{α} is resolved shear stress, and m is the strain rate sensitivity exponent. Equation (5) calculates the shear strain on each slip system contributed by each discrete slip event. Equation (6) is used to evaluate the shear strain rate for each active slip event. The model uses the ratio of these two variables to determine the time taken for the slip event. At the time the slip event completes, a new CRSS is assigned in its place.

Before moving on, a few items on the formulation presented thus far are worth noting. There are more sophisticated forms than Eqn. (4) for the critical stress to bow out a dislocation from a double-pinned source, such as those accounting for screw/edge character dependent line tension, inertial effects, temperature or strain rate, and elastic anisotropy, (Brown, 1964, 2006; Cai and Nix, 2016). These advanced forms can be used in place of Eqn. (4) without altering the

basic approach and size effects, although they would undoubtedly quantitatively affect the stress levels. Secondly, most models calculate a back stress from a pile up onto its source and use this to explain size effects (Meyers et al., 2006; Saada, 2005).

It is worth mentioning that the stress and strain fields at the GB differ from those in the interior of the grain. These can be seen in many other CPFE calculations (Chandra et al., 2018; Lim et al., 2011; Niezgoda et al., 2014). In our model, we did not finely introduce many elements per a grain, but instead have one element per grain. We realize this assumption makes for a simplistic mesh. In doing so, the stress tensor calculated for the element is the stress we use for the dislocation source to expand the dislocation in the grain interior onto its habit plane and propagate it across the element. Thus, it is the "grain average" stress tensor that we use to find the RSS to compare with the CRSS and not the local stress at the GBs to compare with the CRSS. Further, the CRSS is viewed as a propagation stress and not a nucleation stress. Specifically, in the model CRSS is formulated to be the critical stress to critically bow a pre-existing GB dislocation and have it glide across the grain, and is not for the nucleation of dislocation the source. For a nano-grain, this assumption is consistent with the finding from atomistic simulations that the activation barrier for dislocation propagation is larger than that for dislocation nucleation (Bitzek et al., 2008). This assumption would not be valid for a coarse-grain.

In the present development, no back stress is generated due to the immediate annihilation of dislocations upon crossing the grain and reaching the GBs. In actuality, deposited dislocations in the interface may generate back stress. In principle, the backstress can be implemented into the model and applied to study MNCs in cyclic loading. The reverse motion of dislocations may depend on the so called "sink strength" or efficiency of the interface. In nanolayered structures,

if the threading dislocation has not been fully absorbed by the interfaces, it may glide back during the unloading stage in the cyclic test to minimize the dislocation line energy in the material systems. This action could likely induce detectable Bauschinger effects. If the interface, on the other hand, can absorb the dislocations, the driving force to move the dislocation back will be low. In that case, the Bauschinger effect may not be detectable. Last, the formulation presumes that full dislocations are moving across the grain, which do not leave stacking faults, and not partial dislocations for which a stacking fault would trail behind the moving partial. This assumption is adequate for a BCC metal, such as Nb, but may not be appropriate for an FCC metal, like Cu. Many of these aspects can be incorporated into the present model in a straightforward manner, but as this is the first presentation of the two-phase model, we resist further upgrades of the model in the present study.

2.3 The statistical model for boundary dislocation source length

In this model, as mentioned earlier, dislocations are presumed to emanate preferably from the GBs and not the biphase interfaces. The MNC being modeled is comprised of NC layers of Cu and Nb, and as motivated by recent MD simulations, the weaker dislocation sources are assumed to lie within the intralayer GBs, as well as the intersection lines (or triple junctions) where GBs and interfaces meet (Huang et al., 2017). In these same MD simulations, dislocations were observed to also protrude from the biphase interfaces but often at sites where dislocations had impinged on the interface from the other crystal and after some amount of strain, when many dislocations had already propagated from the GBs.

The thickness of the layer h will limit the maximum segment length L of the sources. As illustrated in Figure 1, in order for a dislocation to propagate on a slip plane, the line of the

dislocation segment L must lie along from the intersection line between the slip plane and grain boundary GB (Beyerlein et al., 2013; Huang et al., 2017; Mendelson, 1969). Within the intersection line, the source length L will likely vary statistically, from a minimum value L_{min} to a maximum L_{max}. The minimum source length L_{min} can physically be no shorter than the core of a dislocation and is set equal to (er_0), where e is the base of the natural logarithm and r_0 is the dislocation core size (Peter M. Anderson et al., 2017). The largest source length L_{max} can be no longer than the length of each intersection line, λ, which is given by $\frac{h}{Sin\theta}$, where h is the layer thickness, and θ is the angle between the intersection line and the interface plane. Here we set $L_{max} = a\lambda$, where a is a non-negative constant of order one and can be treated as a roughness parameter. At the length scale of 0.1 to 1 nm of a single dislocation, GBs are rarely planar and are normally curved or faceted, which would be reflected in $a < 1$. In what follows, we set a equal to 0.4.

2.4 Model microstructure and application to Cu/Nb MNCs

The model is applied to recent experiments performed by Nizolek *et al*. (Nizolek et al., 2015). Uniaxial compression tests were carried out on two-phase Cu/Nb MNCs with individual layer thicknesses ranging from 140 nm to 15 nm and in two different in-plane directions, along the rolling direction (RD) and transverse direction (TD) (Nizolek et al., 2016). They found that as the nanolayer thickness decreased, the composite yield strength and the flow stresses increased. They exhibited a strong in-plane TD vs. RD anisotropy.

These MNCs were made by accumulative roll bonding (ARB). The ARB process involves repeated rolling deformation. Within the ARB sheet, both Cu and Nb phases developed a specific, highly oriented deformation texture (Beyerlein et al., 2014a). The Cu/Nb interfaces

also developed a preferred interface character {112}Cu||{112}Nb with a Kurdjumov-Sachs orientation relationship (Beyerlein et al., 2014b). Nanograins in the MNC material were highly elongated in the rolling direction with variable aspect ratios of 30 to 80 times the layer thickness (Carpenter et al., 2013).

The CPFE model of the MNC microstructure is built to mirror the as-processed microstructure before compression testing. The model MNC consists of an alternating stack of the pure FCC Cu with the pure BCC Nb in equal amounts. A separate model is built for every value of h in the experiment and using the corresponding initial texture measured for that layer thickness, although these did not vary appreciably with h. The orientations of the grains within each phase are randomly selected from them. Figure 2 shows one of the measured initial textures, which was replicated in the model. We tested the sensitivity of the texture representation with the number of elements and found that as long as the number of elements was over 1000, the texture could be well represented. This outcome is largely a consequence of the strong texture we are using. As in the actual material, paired Cu and Nb crystals at the interfaces in the model are oriented such that their orientation relationship is Kurdjumov-Sachs and mutual interface plane is a {112}-type plane.

In this application of the model, the Cu/Nb nanolayered composites contain equal volume fractions of Cu and Nb. Each layer consists of 20×20×10 grains with each grain having same grain aspect ratio of 1:20:2 (ND:RD:TD). Symmetric boundary conditions are imposed on the model, wherein the −x, −y and −z surfaces are constrained from moving along the x, y and z directions, respectively, while the + x, + y and +z surfaces are free to move. A uniaxial constant strain rate 0.001 s^{-1} equal to the experiment test strain rate is applied on the RD (+x surface) and TD (+y surface) directions, respectively, to study the RD-TD plastic anisotropy in Cu/Nb

nanolayered composites. As before, we checked the sensitivity by repeating some select simulations with up to four times the number of elements representing the layer. We found that the stress-strain curves are the same. Further, the simulation deforms the MNC model nanostructure up to 4% engineering strain, and for this small strain level, the mesh does not become highly stretched or distorted.

It is important to mention that unlike standard CPFE models, in the present discrete slip version, all the parameters used in the flow rule are measurable and can be easily assigned. Three parameters have been mentioned: the elastic moduli, the reference shear strain rate, $\dot{\gamma}_0$ and strain-rate sensitivity exponent, m. The moduli for Cu and Nb are obtained from measurements of their bulk value (Bolef, 1961). For the Cu and Nb studied here, C_{11} equals 168.4 GPa for Cu and 246.0 GPa for Nb, C_{12} equals to 121.4 GPa for Cu and 134.0 for Nb, and C_{44} equals 75.4 GPa for Cu and 28.7 GPa for Nb. We set the value of reference shear strain rate equal to the experiment test strain rate, 0.001 s^{-1}. The value of m is set to be 0.1, which is the standard value used in conventional crystal plasticity models.

The model uses the preferred slip mode of Cu, the 12 {111} <110> slip systems, and the two preferred slip modes of Nb, the 12 slip systems in the {110} <111> mode and 12 slip systems in the {112} <111> mode. The orientations of all the planes of these systems within representative Cu and Nb crystals are illustrated in Figure 1. The model material parameters for calculating τ_{CRSS} consist of the isotropic equivalent shear moduli and Burgers vector, which are μ = 48.3 GPa and b = 0.2556 nm for Cu and μ = 37.5 GPa and b = 0.2853 nm for Nb. Dislocations in Cu have a wider core than those in Nb, and so for the core radii, we use $r_0 = 5b$ for Cu and $r_0 = 2b$ for Nb. In practice, the variables, A and r_0, may be adjusted within a

reasonable range to better reproduce the experimental stress-strain response. Yet, in this work, we assign them *a priori* and do not adjust them for fitting purposes.

Figure 3 (a) and (b) shows, respectively, the source length and τ_{CRSS} distributions for a particular slip system in $(211)[\bar{1}11]$ Nb and $(111)[01\bar{1}]$ Cu and for a few selected layer thicknesses h. These examples demonstrate that the layer size affects both the average value (mean) and dispersion in the calculated τ_{CRSS} distributions. As h decreases, not only does the average τ_{CRSS} increase, but also the spread in the possible values of τ_{CRSS}. These distributions are slip-system orientation dependent and thus every slip plane for a given MNC with h has its own τ_{CRSS} distribution. Due to their differences in orientation, Burgers vector, and moduli, the τ_{CRSS} values in the distributions in Cu are lower than those for Nb. Last, the distributions for the source lengths for other layer thicknesses carry a similar shape, since they originate from the same basic assumption that all dislocations nucleate from the intersection lines between the slip plane and GBs.

Initially, before loading, all slip systems are assigned a particular τ_{CRSS} at random from their corresponding probability distribution. During the deformation, once the resolved shear stress (RSS) on a specific slip system is larger than CRSS, the dislocation on that slip system will be activated. After the dislocation glides across the nanograin, another source is envisioned to take its event, a new τ_{CRSS} is selected again at random from the probability distribution.

3. Results and discussion

3.1 Comparison between the predicted and measured stress-strain response in two different loading directions

Figure 4 (a) compares the stress-strain curves of Cu/Nb nanolayered composites at two different loading directions (RD and TD) from our prediction and the experiment results (Nizolek et al., 2016) at four different thickness h = 15 nm, 30 nm, 65 nm and 140 nm. The calculated stress-strain responses predict that the MNC flow strengths scale inversely with h and exhibit noticeable plastic anisotropy between TD and RD, in agreement with the experimental measurements. As observed, the calculated strengths under the TD loading direction are higher than those for RD loading direction in layer thicknesses, and more importantly, the difference between the RD and TD stress increases as the layer thickness decrease. While the agreement over the entire flow stress-strain response is not exact, it is reasonable considering that the model outputs are predictions, without use of adjustable parameters to fit these curves. Based on their consistency at the macroscale, these calculations are used to gain further insight into which mechanisms, operating at the microscale, are responsible for the size effect, plastic anisotropy, and strain hardening.

3.2 Layer size scaling of strength

One of the most outstanding mechanical properties of metallic nanolayered composites is the strong strength dependence on layer thickness h. For coarse-grained polycrystalline metallic materials, the Hall-Petch scaling is often used to describe the effect of grain size on yield strength as $\sigma = \sigma_0 + kD^{-1/2}$, where σ is the yield stress, σ_0 the friction stress, k the Hall-Petch slope, which is material dependent, and D the average grain size (Armstrong, 2014). In the case of nanolayers, in which one grain spans the thickness, $h = D$. When the layer thickness, h, is used in place of grain size D, Nizolek *et al*. (Nizolek et al., 2016) showed that the measured yield strengths of the Cu/Nb nanolaminates exhibited a Hall-Petch scaling. Figure 4(b) is a Hall-Petch

plot that compares the 0.2% offset yield strength predicted by the model with their experiment results. Significantly, in agreement with the measurements, the calculated yield strengths follow the Hall-Petch scaling in h.

Since the Hall-Petch size scaling in strength emerges from the calculations, and is consistent with the experiment, the model could help to reveal its origin. The classic explanation for the Hall-Petch relationship involves a dislocation pile-up scenario (Armstrong, 2014). The present model, however, does not consider pile ups or dislocation accumulation within the grains. As mentioned in the introduction, for MNCs, a popular strength model is the confined layer slip (CLS) model (Cao et al., 2019; Liu et al., 2013; Misra et al., 2005; Zbib et al., 2011; Zhang et al., 2017). However, the CLS model only defines the stress required to thread a single dislocation through a layer as a function of h (e.g., $\tau_{CRSS} = \log(h)/h$), but not the finite amount of glide associated with it. In the present model, none of the variables affecting strength, such as source length L or emission stress τ_{CRSS}, had an explicit dependence on layer thickness h. The stress τ_{CRSS} in Eqn. (4) bears a $\log(L)/L$ dependence but not a $L^{-1/2}$ dependence that would resemble the observed macroscopic size scaling [*]. The model identifies that the main sources of the layer size effect are the limit h places on 1) L, length of dislocation sources in the boundary, or more generally, on the range of possible stresses needed to emit and sustain glide of a dislocation from one interface to another and on 2) the discrete amount of shear strain a slip event can provide.

3.3 Role of statistical strength on plastic behavior of MNCs

[*] We also fit the scaling law to h^{-n} with general exponent n. The values for n are -0.43 and -0.46 for the TD and RD cases, which are reasonably close to 0.5, indicating still an emergence of a Hall-Petch effect.

An important feature in the Cu/Nb MNC response, in which the model and experiment coincide, is the strain hardening in the deformation response. In coarse-grained metals, strain hardening is conventionally associated with the multiplication and accumulation of dislocations within the crystals. In very fine h = 10 nm to 100 nm nanolaminates, however, such subgranular dislocation density storage is neither expected nor is it included in the model. The model, however, includes resistances to expanding a GB source, which could be identified as another mechanism for strain hardening. To gain insight into the role of statistical emission, we first, repeated the deformation simulations for h = 30 and 140 nm with the same parameters and initial texture, but with the spatially random variation in CRSS removed and a deterministic (mean) value of τ_{CRSS} used in its place. The corresponding stress-strain curves for thickness of 30 nm and 140 nm (referred to as the "deterministic" case) are also given in Figure 5. Regardless of the layer thickness, the deterministic cases exhibit noticeably less strain hardening and higher yield stresses than the corresponding statistical cases. These differences from the actual stress-strain responses would suggest that the latter are determined by the relatively weaker sources and that the statistical randomness played a part in strain hardening.

In this regard, in simulation, there are two statistical aspects: one spatial and one temporal. Next, simulations were performed with only the temporal (or strain) variation in the CRSS removed, which is accomplished by assigning an initial spatial variation in τ_{CRSS} for the slip systems in all grains and maintaining it, rather than replacing it with a new τ_{CRSS} after completion of every discrete slip event. The corresponding stress-strain curves for this "strain-independent" case are also given in Figure 5. The strain-independent curves exhibit the lowest strain hardening and strength during plastic flow. The outcome indicates that the temporal variation in τ_{CRSS} gives rise to the strain hardening seen in the calculated stress-strain curves.

Weaker sources are activated first, and being the relatively weaker ones, the likelihood is, therefore, high that the next source activated in the same grain will be harder.

3.4 Size effects in the number of discrete slip events

The slip activity associated with the deformation response can be analyzed with respect to not only crystallographic orientation (Schmid factor), as is usually done, but also to layer size h. Figure 6 compares the total number of slip events that occur up to 4% strain in two samples with vastly different layer thicknesses h = 30 nm and 140 nm. The number of slip events scales with the layer thickness, being 4-5 times larger for the 140 layered composites than the 30 nm layered composites. This size scaling in the number of discrete slip events is a consequence of the effect that layer size has on the amount of shear strain per event, $\gamma_{discrete}$. A dislocation gliding in a larger grain contributes less shear to grain deformation than the same dislocation gliding in a smaller grain. In Figure 7, we plot the average value of $\gamma_{discrete}$ for the top ten active slip systems in the Cu and Nb crystalline layers versus h. As shown, $\gamma_{discrete}$ decreases as h. The amount of glide also depends on the geometrical relationship between the GBs and slip planes that are activated. From the analysis in Figure 6, $\gamma_{discrete}$ is smaller for slip events active in the TD test than those active in the RD test.

The analysis in Figure 6 indicates that slip activity is influenced by the both orientation with respect to the loading direction, reflected in the Schmid factor, and the randomness in the τ_{CRSS} for dislocation expansion. The range of Schmid factors theoretically spans 0 to 0.5, but the ranges shown in Figure 6 are narrower, reflecting the sharpness of the initial texture of the material. Generally, we find a weak but non-negligible dependence of the number of discrete slip events on Schmid factor. In all cases, more slip events occur on systems with the higher Schmid

factor. This explains why the TD-RD anisotropy prevailed for all layer thicknesses, despite the spatial and temporal randomness in the τ_{CRSS} to activate slip. The dependence is no stronger for the finer layer thickness h = 30 nm than the coarser one, h = 140 nm. Thus, the growing TD-RD anisotropy is not due to a stronger dependence on texture as the layer h refine but due to the growing increase in the τ_{CRSS} required to cause a discrete slip event.

Figure 6 reveals that the underlying slip involved multiple slip, in which grains did not activate only one slip system, and that all slip systems with non-zero Schmid factor were active at some point in the deformation response. This dispersion in slip amount multiple systems, and non-negligible slip activity on even the relatively low Schmid factor slip systems are outcomes of the statistically varying τ_{CRSS} .

3.5 Effect of layer thickness on the plastic anisotropy

A question that arose earlier concerns the observed layer size effect on plastic anisotropy. Nizolek et al. (Nizolek et al., 2015) demonstrated using a polycrystal plasticity model that the higher flow stress in TD compared to that in RD was attributed to preferred crystallographic texture in the material before testing. Yet, why the TD-RD anisotropy exhibited a layer size effect, increasing inversely with h, could not be addressed with the type of model they used. Here, in Figure 4(c), we compare, as a measure of plastic anisotropy, the difference in strengths in TD and RD at 4% strain (when the material is clearly deforming plastically) from the measurement and our calculation. The model predicts not only the TD-RD anisotropy, but also the layer size effect in the plastic anisotropy observed in the experiment. The h size-dependent anisotropy arises from the individual size scaling of the TD and RD flow stresses. Since the flow

stress and yield stresses follow a Hall-Petch scaling, their difference (σ_{TD} - σ_{RD}) will also scale with $h^{-1/2}$.

3.6 Mechanisms: analysis of activation volumes

Analysis of the activation volume V associated with a plastic response is often used to identify the dominant deformation mechanism. It can be measured by strain rate jump tests (Wang et al., 2006), wherein $V = \frac{\sqrt{3}kT}{m\sigma}$, where m is the strain rate sensitivity, σ is the flow stress, k is Boltzmann's constant and T is the absolute temperature. In coarse-grained polycrystalline metals, the activation volume is associated with dislocation cutting of forest dislocations or particles and is on the order of (~1000·b^3) (Jia et al., 2003; Wei et al., 2004). In nanocrystalline metals, V is typically (~10b^3), two orders of magnitude smaller. The substantial reduction in the activation volume indicates a transition in deformation mechanisms to grain boundary or interface-affected flow, such as GB sliding and migration, dislocation nucleation, and confined layer slip (Yamakov et al., 2003).

In the present model, the activation volume associated with the activation of dislocations in the GBs can be directly evaluated by $V = l \cdot b^2$, where l is the average source length of activated dislocations during plastic flow in our calculations. Figure 8 shows the effect of layer thickness on the activation volume in the Cu phase of the model Cu/Nb nanolayered composites. The values range from $40b^3$ to $110b^3$, signifying interface-affected dislocation motion. A reduction in activation volume is seen with decreasing layer thickness. Although not an especially direct comparison, Figure 8 also includes experimentally determined activation volumes reported for materials with similar chemical composition and grain sizes are shown: the NC Cu (Chen et al., 2006), nanotwinned (NT) Cu (Lu et al., 2009) and ARB Cu/Nb pillar compression tests (Snel et

al., 2017). Collectively, the activation volumes from experimental data are seen to also increase with layer (or twin) thickness. The predictions lie above the activation volumes for UFG Cu, NT Cu and Cu/Nb pillar at 400˚C, but are close to the data for the Cu/Nb pillar at 25˚C, especially for a layer thickness below 100 nm, which correspond to the conditions and material system for which the model is currently applied. The comparison provides some validation of the governing dislocation mechanism of dislocation emission from GBs used in the model.

3.7 Discussion on discrepancies

In Figure 4(b), some discrepancies are clear between the Hall-Petch slopes in yield strength versus layer thickness. The measured k slopes were 3.10 and 3.25 GPa•nm$^{-1/2}$ in the RD and TD loading directions, respectively, whereas the corresponding calculated k values are 1.95 and 3.98 GPa•nm$^{-1/2}$. Arguably, these quantitative differences could easily have been expected, given the lack of adjustable parameters and the idealized microstructure. For the initial microstructure, we sampled from the experimental initial texture and assumed a uniform layer thickness, grain shape and grain size as the input for our calculations. In actuality, the layer thicknesses and grain size vary statistically within the experimental ARB sample after severe plastic deformation.

In the anisotropy in Figure 4(c) and activation volumes in Figure 8, an overestimate is seen, particularly for the large layer thickness samples (h > 100 nm). The model considers only one source for dislocation nucleation, the interface/GB junctions, whereas in actuality there are many other defects in the material that may serve as dislocation sources. This difference can be attributed to the increasing number of non-GB sources of dislocations (intragranular defects) that are introduced when the grain size increases above 100 nm and are not taken into account in the model.

We should recall that as the dislocation thread through the layers, dislocations are deposited in the interface and from there, they could nucleate dislocations or be recovered with dislocations deposited from dislocation threading in adjacent layers. The accumulation of dislocations in the interface and possible role in promoting dislocation nucleation from the interface have been neglected in the present model. Further studies are needed to explore the interface dislocation accumulation in MNCs. At present, experimental evidence of deformed MNCs show relatively clean interfaces with only intrinsic misfit dislocations (Beyerlein et al., 2014b; Zheng et al., 2013; Zheng et al., 2014) and no significant dislocation accumulation on Cu/Nb interfaces. Also, unlike interface nucleation, dislocation storage is not a widely studied topic in atomistic simulations (due to lack of diffusive time scales). If the interface can recover deposited interface dislocations, then interaction of mobile dislocation with deposited dislocations may not be the major contribution for the strain hardening in the Cu/Nb system. In this work, we aimed to demonstrate that layer-limited dislocation sources can capture the main size effect as well as other features of the deformation response, with little to no adjustable parameters. A worthy extension of the present model, however, would be to incorporate interface-driven mechanisms, such as dislocation accumulation in the interface. Like most hardening models this effort may involve introducing phenomenological hardening models that commonly would introduce a few adjustable parameters.

The approach taken for this discrete slip crystal plasticity model is sufficiently fundamental that it can be applied to understand size effects in the deformation response of nanolayered systems with other metallic phases and other crystal structures, such as cubic/cubic or cubic/non-cubic structures. In order to calculate the deformation response these systems, the input for this model are measurable quantities, such as the initial texture, layer thickness, grain

sizes and elastic properties, and applied boundary conditions. In addition, our model can also be implemented into the mean field approaches (Carpenter et al., 2014; Gu et al., 2019) to predict the deformation in MNC, in which the grain-to-grain and phase-to-phase interfaces should be tuned. Similar methods to account for the limits crystallographic twin or interface boundaries impose on the mean free path of dislocations, and local fluctuations of stresses at the grain boundaries have been implemented in such techniques in previous works (Beyerlein et al., 2011; Chelladurai et al., 2019; Kumar et al., 2017).

4. Conclusions

In summary, we present a crystal plasticity finite element model for metallic nanolayered composites (MNCs) that accounts for the layer thickness effect on composite constitutive response by incorporating a statistical dislocation source model for the activation of slip. In this model, plasticity occurs in the nanocrystalline layers of the composites by discrete slip events, gliding from grain boundary to grain boundary. We show that the predicted stress-strain curves and the plastic anisotropy agree well with the experimental measurements, without use of adjustable parameters. Moreover, a Hall-Petch scaling arises in the model predictions and is explained based on the limits layer thickness places on the dislocation source lengths. We show that a coupling exists between the texture and layer size that gives rise to size effects on plastic anisotropy. This work benefits understanding of the plastic anisotropy observed in Cu/Nb nanolayered composites and can shed light on the role of dislocation mechanisms in the mechanical response of MNCs.

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