A multi-scale model for texture development in Zr/Nb nanolayered composites processed by accumulative roll bonding

M Ardeljan¹, M Knezevic¹, T Nizolek², I J Beyerlein³, S J Zheng⁴, J S Carpenter⁵, R J McCabe⁶, N A Mara⁴ and T M Pollock²

¹ Department of Mechanical Engineering, University of New Hampshire, Durham, NH 03824, USA
² Materials Department, University of California at Santa Barbara, Santa Barbara, CA 93106, USA
³ Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
⁴ Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
⁵ Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

E-mail: marko.knezevic@unh.edu, irene@lanl.gov

Abstract. Recently it has been demonstrated that nanolayered hcp/bcc Zr/Nb composites can be fabricated with a severe plastic deformation technique called accumulative roll bonding (ARB) [1]. The final layer thickness averaged to approximately 90 nm for both phases. Interestingly, the texture measurements show that the textures in each phase correspond to those of rolled single-phase rolled Zr and Nb for a wide range of layer thickness from the micron to the nanoscales. This is in remarkable contrast to fcc/bcc Cu/Nb layered composites made by the same ARB technique, which developed textures that strongly deviated from theoretical rolling textures of Cu or Nb alone when the layers were refined to submicron and nanoscale dimensions. To model texture evolution and reveal the underlying deformation mechanisms, we developed a 3D multiscale model that combines crystal plasticity finite element with a thermally activated dislocation density based hardening law [2]. For systematic study, the model is applied to a two-phase Zr/Nb polycrystalline laminate and to the same polycrystalline Zr and polycrystalline Nb as single-phase metals. Consistent with the measurement, the model predicts that texture evolution in the phases in the composite and the relative activities of the hcp slip modes are very similar to those in the phases in monolithic form. In addition, the two-phase model also finds that no through-thickness texture gradient develops. This result suggests that neither the nanoscale grain sizes nor the bimetal Zr/Nb interfaces induce deformation mechanisms different from those at the coarse-grain scale.
1. Introduction

Two-phase metal-metal nanolayered composites have much to offer in developing scientific understanding of interface effects and in creating novel metals with extraordinary properties than those currently in use. These nanomaterials consist of two dissimilar, immiscible metals, where one or both metals have nanoscale dimensions. Earlier research on nanolayered composites focused on small-scale thin film composites made by bottom-up processing such as deposition techniques [3-11]. More recently, studies have probed bimetal interfaces/defect interactions under mechanical and radiation conditions [10, 12, 13]. In efforts to scale up such nanomaterials so that large-scale structural applications can take advantage of their excellent properties, researchers have been employing top-down severe plastic deformation (SPD) techniques. Using SPD, it is possible to make large-scale (bulk) composites of similar composition and architecture as the deposited thin films. Prior works on SPD bimetal composites have focused on systems containing face centered cubic (fcc), body-centered cubic (bcc), and hexagonal close packed (hcp) phases: Cu/Ag [14, 15], Cu/Nb [16-20], Al/Zn [21], Cu/Ni [22], Ag/Fe [23], and Zr/Nb [2, 24, 25]. Significantly, it has been recently reported that like the deposited films, these SPD processed composites possess high hardness, excellent radiation resistance, good shock resistance and outstanding thermal stability [11, 18, 26-29]. Advantageously, unlike the films, composites made by deformation processing have the potential to serve as robust materials in structural applications. Furthermore it has been recently demonstrated that their interface character can be altered by redesigning the processing pathway [30].

The SPD processing invokes substantial changes in microstructure, such as texture, grain shape, grain boundary properties, bimetal interface and internal grain dislocation storage [16, 19, 24, 27, 31-34]. The post-deformation behavior (strength, ductility, failure behavior) and anisotropy in these properties depend on microstructure. The SPD of bimetal composites also enables refinement of the microstructure to nanoscale dimensions. The combination of large strain behavior and plasticity at the nanoscale is a regime that has not been extensively explored for bimetal systems, apart from texture studies on wire-drawn and rolled composites [17, 19, 20, 27, 32, 35].

Recently both 50/50 Cu/Nb and Zr/Nb nanolayered composites were fabricated via the same SPD technique called accumulative roll bonding (ARB) [1, 27, 30]. Both composites formed sharp bimetal interfaces despite the large strain deformation. Also the reduction in layer thickness in both composites remained consistent with the applied rolling reduction through the processing steps, indicating that both layers co-deformed plastically. When refining the individual layer thicknesses from micron-sized layers to nano-sized layers, the textures in the Cu/Nb phases (submicron and below) strongly deviated from those expected when the Cu and Nb are rolled alone [17, 27]. However, the textures in the Zr/Nb composites did not appear to deviate appreciably [1]. The textures in the Zr and Nb phases in the composite at all layer thicknesses were similar to the rolling textures found in literature in the corresponding monolithic materials after large strains.

As a first step in explaining the latter result on Zr/Nb, in this article, we use a recently developed 3D multiscale crystal plasticity finite element-dislocation density based model (DD-CPFE) [2] to predict texture evolution under large strain deformation and while enforcing co-deformation in the presence of a bi-metallic interface. The model has several unique features: treatment of large-strain deformation involving hundreds of percent strain; calculation of the coupled evolution of dislocation density and texture; local stress and strain fields; grain-interface interactions in co-deformation; and grain-grain interactions within the
layers. The latest is best revealed when the grain structure is explicitly represented [36]. The predicted textures for the single-phase Zr and Nb rolled alone and the rolled two-phase composites were the same and agreed well with the measured deformation textures reported in the literature for each phase in the two-phase composite and for each phase rolled alone. Based on the consistency between the experimental and simulation results, we conclude that the co-deformation at the interface did not affect bulk texture development in the Zr/Nb composite fabricated by ARB. The interesting implications are that 1) neither the nanoscale grain sizes nor the bimetal Zr/Nb interfaces induce deformation mechanisms different from those at the micron-scale and 2) dislocation-mediated plasticity accommodates deformation in the Zr/Nb SPD composites when refining the layer thicknesses from 100 µm to 0.1 µm.

This article is structured as follows. We first review some experimental details on materials and processing [1, 25] and present the multiscale model, ending with a characterization of material parameters. Next we discuss texture evolution seen experimentally and compare the measurements with predictions from our model. We end with the implications of these results.

2. Accumulative roll bonding

2.1 Starting materials

We started with 1 mm thick plates of high-purity Zr with nominal composition expressed in weight parts per million (Wt. ppm) Hf <35, Fe <50, Al <20, V <50, O <50, N <20, C <22, Zr balance [37] and a reactor grade high-purity Nb (99.97% pure, ATI-Wah Chang) with composition (Wt. ppm) C<20, Fe <25, H <3, Hf <30, Mo <30, N <20, Ni <20, O<40, P<30, Si<25, Ta=110, Ti<30, W<30, Zr<30 and Nb balance.

The as-received Zr was prepared by a proprietary process. Before we received it, we only know that the Zr was initially upset forged, subsequently clock-rolled and annealed at 550 °C for 1h. This produced a strongly textured plate, whose normal direction is nearly aligned with the c-axis. After receipt, we rolled the material at room temperature to 60% reduction and annealed it at 600 °C for 1h. Figure 1 shows the final grain microstructure and texture of the Zr. The grains are equiaxed, twin-free, and ~ 40 µm in size. The material has a strong basal texture, with the basal poles slightly tilted towards the transverse direction (TD).

The as-received Nb was deformed to 30% rolling reduction and subsequently annealed at 950 °C for 1 h. The resulting Nb exhibited a (111) fiber texture and had a 300 µm average grain size (Fig. 1).
Figure 1. EBSD orientation maps showing the initial microstructure and texture of the as-annealed sample of rolled Zr and Nb. The colors in the orientation maps indicate the orientation of the ND sample direction with respect to the grain orientations [25].

2.2 SPD processing

ARB was then used to fabricate Zr/Nb layered composites from the sheets of Zr and Nb. In preparation for ARB processing, the annealed Zr and Nb sheets were ultrasonically cleaned in a bath of acetone and wire-brushed. For the rolling, we used a 2-high rolling mill (Waterbury-Farrel, Brampton, Ontario, Canada) at Los Alamos National Laboratory. All rolling took place at room temperature and quasi-static rates. The first step involves conventional rolling, where the two sheets were alternately stacked and roll-bonded together at room temperature using a single high-strain rolling pass of approximately 60% reduction. Unlike conventional rolling, ARB involves repetitive cutting, restacking, and rolling steps. Accordingly, the first Zr/Nb bonded material was subsequently cut in half and the process of surface cleaning, stacking, and roll bonding was repeated. Every two rolling passes, the sample was annealed [for more details see Ref. 1]. With each rolling pass the strains accumulated and the individual layer thicknesses refined.

Using this technique, micro- to nano-layered Zr-Nb composites were fabricated. Figure 2 shows some examples of the resulting Zr/Nb layered microstructures, from average layer thicknesses of 210 µm, 28 µm, 4 µm, to 90 nm. The main obstacle to creating a composite with uniform nanometer-scale layers is the development of shear bands (Fig. 2a). The
annealing steps between rolling passes minimized shear banding and therefore facilitating further refinement (Fig. 2b and c) [1].

As shown in Figure 2 the interfaces are not planar and take on an undulating morphology. The deviation from planarity is also observed in ARB Zr/Nb layered composites made without intermediate annealing [25] and in Cu/Nb layered composites [29]. It has recently been demonstrated that upon heating into the (αZr) + (βZr, Nb) two phase area within the Zr-Nb phase diagram that complete wetting of the Nb/Nb grain boundaries by Zr occurs [38]. In this Zr-Nb study, the annealing treatment used (575°C for one hour) has a temperature below what is required to achieve the two phase region (620°C) where wetting is known to occur. The transformation from a flat to roughened interface under rolling has been predicted in CPFE modeling of Cu/Nb multilayers [39, 40]. As shown later, our present model also predicts roughening. Continuum based models suggest that this instability is due to disparate flow stresses and hardening rates between the two phases [41].

Figure 2. Lamellar microstructures in the Zr/Nb composite produced by the ARB process (a) optical micrographs showing the material processed without annealing to layer thicknesses of 210 µm, 28 µm, and 4 µm [25], (b) an optical micrograph showing the material processed with annealing every other rolling pass with 4 µm layer thickness, (c) TEM micrograph showing layer thicknesses of 90 nm, taken from [1].
3. Multi-scale modeling method

The multiscale model is illustrated in Fig. 3. The subcomponents shown are described in turn below.

![Figure 3. Multiscale modeling framework for linking sub-grain physics of deformation and polycrystalline response.](image)

3.1 Micromechanical finite element Zr/Nb model

The overall response of the polycrystal is obtained by a micromechanical finite element model. In this approach, a finite element mesh contains finite elements representing the crystalline metal. Each integration point in a finite element of this mesh corresponds to a crystal lattice orientation.

Figure 4 shows the 3D single-phase Nb, single-phase Zr, and two-phase Zr/Nb finite element models in the global 1-2-3 (RD-TD-ND) orthogonal coordinate system. In the composite model, Nb is the top layer and Zr is the bottom one. As each phase is a polycrystal, we used as many elements as necessary to realistically capture the measured initial texture (Fig. 1). The elements were hexahedral (brick) elements, containing eight integration points representing eight grains with distinct orientations. Each phase has 16x16x8 elements, the composite has 16x16x16 elements and the number of crystal orientations for Zr and Nb together is 32768. The interface between Zr and Nb in the composite model is initially flat.

The grains on either side of the Zr/Nb interfaces were kinematically constrained to maintain displacement and traction continuity with all their nearest neighboring grains. Two different realizations were carried out of the same simulation but different samplings from the crystallographic grain orientations of the initial measured texture. The results that follow combine these two to represent the calculated textures.

![Figure 4. Initial FE meshes of Nb, Zr, and Zr/Nb.](image)

For each element, the linearized governing FE equation based on the principle of virtual work is given by:

$$\left( \int_V \mathbf{B}^T \mathbf{J} \mathbf{B} dV \right) \Delta \mathbf{U} = \mathbf{R}^T - \int_V \mathbf{B}^T \mathbf{\sigma} dV$$  

(1)
where $\mathbf{B}$ is the FE strain-displacement matrix, $\mathbf{J}$ is the material Jacobian, $\Delta \mathbf{U}$ is the displacement increment solution field, $\mathbf{\sigma}$ is the Cauchy stress, and $\mathbf{R}$ is any applied forces [42]. The FE code passes information on the deformation gradient $\mathbf{F}$ at the current time, $\tau = t + \Delta t$, and previous time, $t$, the time increment $\Delta t$ and a range of material related state variables, such as dislocation density (section 3.3) and crystal orientation, to the material subroutine. The user-defined material model then provides $\mathbf{\sigma}$, $\mathbf{J}$, and the updated material state variables for each integration point at each time increment. Here we use the ABAQUS platform for the user material subroutine. Below, we describe how the single-crystal constitutive model (section 3.2) and DD hardening law (section 3.3) are incorporated into this subroutine.

### 3.2 Crystal plasticity constitutive law

For each integration point in the micromechanical FE model we employ a crystal plasticity constitutive law [43] to relate material stress $\mathbf{\sigma}$ to material distortion $\mathbf{F}$ (stretch plus rotations). In this law, the material is elastically and plastically anisotropic. We provide a brief summary below and refer the reader to [43-48] for more details.

In the finite deformation formulation we use, the total deformation gradient tensor $\mathbf{F}$ at a material point is decomposed into its elastic $\mathbf{F}^e$ and plastic $\mathbf{F}^p$ components as stated by

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$$

where $\mathbf{F}^e$ is the deformation gradients for both elastic stretching and lattice rotation and $\mathbf{F}^p$ is the deformation gradient for plastic deformation. The gradient $\mathbf{F}^e$ is related to stress by [43]

$$\mathbf{F}^e = \mathbf{C} \mathbf{E}^e, \quad \mathbf{E}^e = \frac{1}{2} (\mathbf{F}^e \mathbf{F}^e - \mathbf{I})$$

where $\mathbf{\sigma}$ is the Cauchy stress, $\mathbf{E}^e$ and $\mathbf{C}$ are work conjugate stress and strain measures, and $\mathbf{C}$ is the fourth-order elasticity tensor. The gradient $\mathbf{F}^p$ is related to crystallographic slip at a material point via:

$$\dot{\mathbf{F}}^p = \dot{\mathbf{L}}^p \mathbf{F}^p, \quad \dot{\mathbf{L}}^p = \sum_{\alpha} \dot{\gamma}^\alpha \mathbf{b}_{\alpha} \otimes \mathbf{n}_{\alpha}, \quad \mathbf{F}^p(\tau) = \left[ \mathbf{I} + \Delta t \dot{\mathbf{L}}^p(\tau) \right] \mathbf{F}^p(t)$$

where $\mathbf{L}^p$ is the plastic velocity gradient; $\dot{\gamma}^\alpha$ is the slip rate on $\alpha; \mathbf{b}_{\alpha}$ and $\mathbf{n}_{\alpha}$ are the slip direction and the slip plane normal of $\alpha$, respectively, in the undeformed configuration; and $\mathbf{I}$ is the identity matrix. The $\dot{\gamma}^\alpha$ is related to the resolved shear stress ($\tau_{\alpha} = \mathbf{b}_{\alpha} \cdot \mathbf{\tau} \otimes \mathbf{n}_{\alpha}$) and characteristic resistance shear stress ($\tau_{\alpha}^c$) of $\alpha$ via a power-law relationship [49]:

$$\dot{\gamma}^\alpha = \frac{\dot{\gamma}_0^\alpha}{\tau_{\alpha}^c} \left( \frac{\tau_{\alpha}^c}{\tau_{\alpha}} \right)^m \text{sign}(\tau_{\alpha}^c)$$

where $\dot{\gamma}_0^\alpha$ is a reference slip rate (taken here as 0.001 s$^{-1}$) and $m$ is a parameter that is related to the strain rate sensitivity. Here $m$ is set to 0.01, a value that applies to most metals at low homologous temperatures.

The lattice spin $\mathbf{W}^*$ is related to $\mathbf{L}^p$ via:

$$\mathbf{W}^* = \mathbf{W}^{app} - \mathbf{W}^p, \quad \mathbf{W}^p = \frac{1}{2} \left( \mathbf{L}^p - \mathbf{L}^p^T \right)$$
where $W^a$ is the spin applied to the polycrystal and $W^p$ is the plastic spin, the skew-symmetric component of $L^\alpha$ (see Eq. (4)).

3.3 Dislocation density evolution

The evolution of the characteristic stresses $\tau_c^\alpha$ of each slip system $\alpha$ is based on the evolution of dislocation density in the grain, where dislocations evolve according to a thermally activated rate law. This physically based dislocation density (DD) model replaces the empirical hardening laws that are sometimes used in CPFE modeling. In prior work, the DD hardening model used here [50] has been successfully applied to a broad variety of metals, differing in crystal structure, such as bcc “Haynes 25” [51], Nb [25], Mg [52], Zr [24, 50, 53], Be [54], and uranium [55-57]. All the foregoing studies implemented the DD model into the mean-field polycrystal visco-plastic self-consistent (VPSC) [50, 58] scheme. As deviation from these works, here we incorporate the DD model into CPFE. The combined 3D DD-CPFE model enables predictions of spatially resolved stress and strain fields based on dislocation density and grain reorientation.

Consistent with experimental observation, the DD model allows for a number of possible slip systems to be activated in Zr and Nb. For Zr, plasticity is potentially carried by prismatic <a> slip, first-order <c+a> pyramidal and basal <a> slip. Prismatic $\{1\overline{1}0\}$ slip is the easiest deformation mode and pyramidal $\{0\overline{1}T\}$ slip relatively harder [59]. Basal slip is not prevalent in Zr for small to moderate strains, but recently found to prevail at larger strains [24, 60, 61], making it a likely active and important slip mode in the ARB process.

For Nb, plastic deformation is assumed to be carried by the $\{110\}$ and $\{112\}$ slip systems. The need for employing these two families of slip for capturing the plastic anisotropy of this metal was elucidated by a combined atomic-discrete dislocation simulation [62]. Several dislocation-based models for BCC metals, like Nb, have been developed to account for strain hardening, substructure development, [63-65] and non-Schmid effects [62, 66, 67]. From these works, it is clear that $\{110\}$ and $\{112\}$ slip dislocations have different slip resistances and dependencies on stress, temperature, and strain rate. As a simplification, here we only attempt to model thermally activated slip in Nb and neglect non-Schmid effects or differences in hardening between these two slip modes. It is fully recognized that incorporating these effects is an important topic for future work.

Because the ARB process is carried out at room temperature, we do not consider deformation twinning in the present constitutive model. Compared to the ARB conditions, deformation twinning in Zr and Nb is pervasive at colder temperatures and higher rates [53, 68]. For Zr, tensile $\{1012\}$ twinning can occur in small fractions at room temperature provided that the applied load and orientation are such that the basal poles experience an extension strain or stress [53, 69]. For Nb, prior experimental characterization of ARB Cu-Nb composites made under the same temperature and rate conditions found that Nb did not twin, even at the finest nanoscale thicknesses [70]. Based on these prior results, we suppress deformation twinning in this work. Texture measurements made on this material after deformation, shown later, confirm that at least at the bulk-scale, texture was not affected by twinning. Whether twinning occurs or not in Zr would require EBSD analyses.

The slip resistance $\tau_c^\alpha$ of each slip system $\alpha$ is given by:

$$
\tau_c^\alpha = \tau_{o,f}^\alpha + \tau_{o,HP}^\alpha + \tau_{for}^\alpha + \tau_{sub}^\alpha.
$$

(7)
where $\tau_{o,f}^a$ is a friction stress (dependent on the Peierls stress, interstitials, precipitates and the initial dislocation density), $\tau_{o,HP}^a$ is the resistance contribution from grain boundaries or twin boundaries, and $\tau_{for}^a$ and $\tau_{sub}^a$ are the resistance contributions respectively from dislocation-dislocation interactions with a spatially random forest of dislocations and with a patterned distribution of dislocations (cell walls, subboundaries, etc). The barrier resistance $\tau_{o,HP}^a$ does not evolve with strain and is related to the average grain size grain diameter $d_g$ via a Hall-Petch relationship:

$$\tau_{o,HP}^a = \mu H^a \left( \frac{b^a}{d_g} \right),$$

where $b^a$ is the value of the Burgers vector, $\mu$ is the effective shear modulus, and $H^o$ is a local “Hall-Petch-like” coefficient (not to be confused with the value obtained from macroscopic tests of the same metal with different grain sizes). The resistances $\tau_{for}^a$ and $\tau_{sub}^a$ evolve with strain, changing as the forest dislocation density $\rho_{for}^a$ and the substructure density $\rho_{sub}^a$ evolve with strain via:

$$\tau_{for}^a = \chi b^a \mu H^a \sqrt{\rho_{for}^a}, \quad \text{and} \quad \tau_{sub}^a = k_{sub} b^a \sqrt{\rho_{sub}^a} \log \left( \frac{1}{b^a \sqrt{\rho_{sub}^a}} \right),$$

where $\chi = 0.9$ is a dislocation interaction parameter, $\mu^a$ is the shear modulus and $k_{sub} = 0.086$ is a mathematical parameter that ensures that Eqn (9) recovers the Taylor law at low dislocation densities. The evolution of the stored forest density $\rho_{for}^a$ is dictated by a competition between the rate of storage and the rate of dynamic recovery:

$$\frac{\partial \rho_{for}^a}{\partial \gamma^a} = \frac{\partial \rho_{gen,for}^a}{\partial \gamma^a} - \frac{\partial \rho_{rem,for}^a}{\partial \gamma^a} = k_1^a \sqrt{\rho_{for}^a} - k_2^a (\dot{\varepsilon}, T) \rho_{for}^a, \quad \Delta \rho_{for}^a = \frac{\partial \rho_{for}^a}{\partial \gamma^a} |\Delta \gamma^a|,$$

where $k_1^a$ is a coefficient for the rate of dislocation storage due to statistical trapping of gliding dislocations by the forest of dislocations and $k_2^a$ is the coefficient for the rate of dynamic recovery, given in

$$\frac{k_2^a}{k_1^a} = \chi \frac{b^a}{g^a} \left( 1 - \frac{kT}{D^a b^3} \ln \left( \frac{\dot{\varepsilon}}{\dot{\varepsilon}_o} \right) \right),$$

where $k$, $\dot{\varepsilon}_o$, $g^a$, and $D^a$ are respectively Boltzmann’s constant, a reference strain rate, effective activation energy, and a drag stress. Dynamic recovery can include many thermally activated processes (junction formation, annihilation). They generally rely on elementary dislocation maneuvers, such as dislocation cross slip and climb, to overcome barriers to dislocation motion and enable removal of dislocation line length. We attribute $g^a$ to the dominant process of all such de-pinning processes, which has a much lower barrier than the rest.
It has been proposed that the same basic processes involving climb and cross slip can also be responsible for pattern formation \[62, 64, 71, 72\]. To represent the connection, the hardening model considers a large fraction of these processes to contribute to recovery of forest dislocations and a smaller fraction to substructure development. Furthermore, it assumes that all active dislocation types can contribute to the evolution of substructure. This leads to the following expression for the increment in substructure density with strain:

\[
\Delta \rho_{\text{sub}} = \sum_{\alpha} q^\alpha b^\alpha \frac{\partial \rho_{\text{rem}}^\alpha}{\partial \gamma^\alpha} \left| \Delta \gamma^\alpha \right|
\]

where \( q \) is a coefficient defining the fraction of an \( \alpha \)-type dislocations that add to substructure.

### 3.4 Jacobian

The Jacobian matrix \( \mathbf{J} \) plays a critical role in the rate of global convergence of the FE governing equation given in Eq. (1) \[42\]. It is given by \( \frac{\partial \mathbf{E}}{\partial \Delta \mathbf{E}} \), where \( \Delta \mathbf{E} \) is the logarithmic strain increment tensor provided by ABAQUS. Newton-type implicit FE iteration method uses the Jacobian matrix for altering the deformation field at each FE integration point \( \mathbf{F} \) in the current strain increment until the current stress \( \mathbf{\sigma} \) satisfies the principle of virtual work. An analytical Jacobian matrix has been rigorously derived for saturation hardening laws of the Voce-type \[73-75\]. For the DD based hardening law we use here, the Jacobian matrix had to be modified. Below we present the modification in terms of \( \frac{\partial \tau_{\alpha}}{\partial \Delta \gamma^\alpha} \):

\[
d\tau_{\alpha} = \frac{\partial \tau_{\alpha}}{\partial \Delta \gamma^\alpha} d\Delta \gamma^\alpha = \frac{\partial \tau_{\alpha}^{\text{for}}}{\partial \Delta \gamma^\alpha} d\Delta \gamma^\alpha + \frac{\partial \tau_{\alpha}^{\text{sub}}}{\partial \Delta \gamma^\alpha} d\Delta \gamma^\alpha
\]

\[
d\tau_{\alpha} = \frac{1}{2} b^\alpha \mu \left[ X\left( k_{1}^{\alpha} - k_{2}^{\alpha} \sqrt{\rho_{\text{for}}^{\alpha}} \right) + k_{\text{sub}} b^\alpha q^\alpha \rho_{\text{for}}^{\alpha} \left[ \ln \left( \frac{1}{b^\alpha \sqrt{\rho_{\text{sub}}}} \right) - \frac{1}{\ln 10} \right] \right] d\Delta \gamma^\alpha
\]

### 4. Model characterization based on uniaxial testing of single-phase materials

There are several material parameters associated with each slip system \( \alpha \): the Peierls stress \( \tau_{\alpha}^{\text{ref}} \), trapping rate coefficient \( k_{1}^{\alpha} \), activation barrier for de-pinning \( g^{\alpha} \), and drag stress \( D^{\alpha} \). Previously, using a VPSC-DD framework and a suite of experimental data, these parameters were characterized for the same three slip modes in Zr and two slip modes in Nb we will consider here \[24, 25\]. Because our multiscale modeling framework is different, we checked these parameters using a simple uniaxial compression test to ensure they are sufficient. For the DD-CPFE model, the starting model microstructures were single-phase polycrystals of either Zr or Nb comprised of 15,000 grain orientations whose texture matched the measured initial texture (see Fig. 1). Axial compression in 0.001 strain increments along the ND sample direction (Fig. 4) was applied, while the two lateral directions (TD and RD) were forced to be stress-free. We find that to achieve the excellent fit shown in Fig. 5, only minor adjustments to the DD material parameters for Zr and Nb reported earlier \[24, 25\] had to be made. Tables I and II list these parameters used hereinafter.
Figure 5. Stress-strain responses of monolithic Zr and Nb in simple compression at room temperature and quasi-static strain rate.

Table 1 Constitutive parameters for evolution of slip resistance in the Zr phase

| α – slip mode | prismatic slip | basal slip | pyramidal slip |
|---------------|----------------|------------|---------------|
| $\tau_{o,f}^\alpha$ [MPa] | 5              | 130        | 105           |
| $k_i^\alpha$ [m$^{-1}$] | 3x10$^7$       | 1x10$^{10}$ | 4x10$^7$      |
| $g^\alpha$      | 3.75x10$^{-7}$ | 3.7x10$^{-2}$ | 2.8x10$^{-2}$ |
| $D^\alpha$ [MPa] | 330            | 300        | 100           |
| $\dot{\varepsilon}_o^\alpha$ (s$^{-1}$) | 10'            | 10’        | 10’           |
| $q^\alpha$ [MPa] | 88             | 0          | 0             |
| $H^\alpha$ [MPa] | 100            | 100        | 170           |

Table 2 Constitutive parameters for evolution of slip resistance in the Nb phase

| α – slip mode | {110} & {112} slip |
|---------------|-------------------|
| $\tau_{o,f}^\alpha$ [MPa] | 94                |
| $k_i^\alpha$ [m$^{-1}$] | 5.2x10$^7$        |
| $g^\alpha$ | 3.5x10$^{-2}$     |
| $D^\alpha$ [MPa] | 230               |
| $\dot{\varepsilon}_o^\alpha$ (s$^{-1}$) | 10’               |
| $q^\alpha$ [MPa] | 14                |
| $H^\alpha$ [MPa] | 50                |

5. Texture evolution in Zr/Nb ARB composites

5.1 Experimental measurement

To measure the crystallographic texture, we used electron backscattered diffraction (EBSD) for the micron samples and neutron diffraction for the nanolayered sample. The EBSD was conducted on an FEI XL30 SEM using a TSL/EDAX EBSD camera and software. The sizes of our high-resolution scans range from approximately 1000 µm$^2$ to 3600 µm$^2$ with
layer reduction and each scan contained at least 600 grains. We only used orientation measurements with a confidence index of 0.3 or more. Neutron diffraction was performed on the HIPPO diffractometer at the Los Alamos Neutron Science Center (LANSCE).

Figure 6 shows the textures for \( h = 210 \mu m, 28 \mu m, 4 \mu m, \) and 90 nm. The larger length scale textures are from the EBSD measurements on materials that were not annealed during processing while the last, 90 nm texture, is from the material that was annealed in-between processing steps. The micrographs show all of the annealed materials. The textures in both phases evolve and sharpen with strain. Remarkably, the textures in the phases do not appreciably deviate from the rolling textures of Zr and Nb in monolithic form [34, 76-80]. For all \( h \) shown, the Zr texture exhibits a strong \((0002)\) texture component, slightly tilted from the normal direction (ND) by 30-50° in the TD direction along the ND-RD plane. This feature, as well as the distribution of the other poles, corresponds well with previous measurements reported for single-phase Zr [34, 76-80].

For Nb, we present the deformation texture evolution in the Nb phase within the composite in the form of pole figures in Fig 7 and in a \( \varphi_2 = 45^\circ \) section in Euler space in Fig. 8. Again, for all \( h \), the Nb textures exhibit a typical BCC rolling texture recognized by two fibers, the \((001)\) \( \alpha\)-fiber and \((111)\) \( \gamma\)-fiber with pronounced \((001)(110)\) and \((111)(110)\) texture components, respectively. These features are also consistent with previous pole figures [81, 82] and orientation distribution function (ODF) sections in Euler space [83-86] reported for rolled single-phase Nb. In addition they are also similar to textures in ARB Cu/Nb composites with micron-thick Nb layers [17, 39].

![Figure 6. Measured pole figures showing the texture evolution in the Zr phase during ARB at strains for layer thicknesses of (a) 210 \( \mu m \), (b) 28 \( \mu m \), (c) 4 \( \mu m \), and (d) 90 nm.](image-url)
Figure 7. Measured pole figures showing the texture evolution in the Nb phase during ARB at strains for layer thicknesses of (a) 210 µm, (b) 28 µm, (c) 4 µm, and (d) 90 nm.

Figure 8. \( \varphi_2 = 45^\circ \) ODF section showing the measured texture in the Nb phase for the following layer thicknesses (a) 210 µm, (b) 28 µm, (c) 4 µm and (d) 90 nm. Level lines correspond to 0.7/1.0/1.5/2.3/3.5/5.3/8.0.

5.2 Model predictions

Evidently, for a wide range of layer thicknesses from the micron to the nanoscale, we find that the texture evolution in the Zr and Nb phases in the rolled composite do not deviate from those reported earlier in the rolled monolithic materials. This observation suggests that the nanoscale crystal dimensions and the Zr/Nb interface negligibly affect bulk texture evolution.
and likely also the deformation mechanisms. As a way of confirming this observation in a
systematic fashion and to assess the corresponding deformation mechanisms, we apply the
DD-CPFE model presented in section 3.0 and simulate texture evolution during rolling in a
single-phase Nb, single-phase Zr, and a two-phase Zr/Nb composite. All the following
predictions were obtained using the single set of hardening parameters presented in Tables I
and II; these parameters were not re-adjusted to fit the ARB texture data.

5.3 Rolling simulation
To model rolling, the 3D polycrystal models in Fig. 4 were subjected to plane strain
compression (PSC). This deformation state best applies to the center of the sheet away from
the surfaces where contact with the rolls can cause additional back and forth shearing. The
velocity gradient tensor associated with PSC in the global 1-2-3 (RD-TD-ND) orthogonal
coordinate system shown in Fig. 4 is given by:

\[
L^{psc} = \begin{bmatrix}
\dot{\varepsilon} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & -\dot{\varepsilon}
\end{bmatrix}
\] (14)

To realize PSC, the boundary conditions are: imposing a strain rate of 0.001/s in strain
increments ranging from 0.005 to 0.01 to all nodes on the top in the negative 3-direction,
constraining the nodes in the bottom face in the 3-direction (ND), constraining the front and
back faces in the 2-direction (TD), leaving the right face free (rolling direction RD), and
constraining the left face in the 1-direction.

To simulate the large strain behavior associated with repeated rolling in the ARB process,
the calculated final texture and dislocation density from the previous rolling pass are used to
initialize the next rolling pass. The simulations followed the experimental schedule where the
first pass imposed a strain of 1.0 and every subsequent pass a strain of 0.5.

5.4 Von Mises stress fields
Figure 9 compares the von Mises stress fields in the deformed structures in these cases.
As shown, the phases in the composite experience considerably less heterogeneity in
deformation, presumably due to load sharing. Notably, the interface is seen to roughen,
consistent with experimental observation (Fig. 9). Apart from roughening, no particular
localization or stress gradients are seen to develop at the interface.
Figure 9. Deformed FE models of monolithic Nb, monolithic Zr and the Zr/Nb composite showing Von Mises contours in [MPa] at strain levels corresponding to layer thicknesses of 210 µm and 4 µm.

5.0 Deformation textures

Figures 10 and 11 compare the predicted deformation textures for both phases alone and in the composite. As in the experiment, whether the phase lies within a composite or alone, the textures are virtually the same. Furthermore, the model predicts well the main texture features consistent with experimental observation (see Figs. 6, 7). For Zr, the basal pole figure shows the characteristic ~20-40° tilted (0002) texture component from the ND direction and towards the TD direction. The (10\bar{1}0) pole figure shows the characteristic alignment with the rolling direction (RD) and formation of maxima at about 60° and 30° from the RD and the TD directions, respectively. For Nb, the model predicts the main peaks associated with the α and γ BCC fibers. These are better illustrated in the $\phi_2 = 45^\circ$ section in Fig. 12. These features are observed in both the micron and nano-scale composite texture measurements.
Figure 10. Calculated pole figures of Zr (a) monolithic (c) in the composite and (d) in the interface region of the composite corresponding to a layer thickness of 4 µm.

Figure 11. Calculated pole figures of Nb (a) monolithic (c) in the composite and (d) in the interface region of the composite corresponding to a layer thickness of 4 µm.
With the DD-CPFE model it is also possible to capture texture gradients between two adjacent Zr/Nb interfaces. Such gradients may not be realized in a bulk texture measurement but can be accessed via spatially resolved techniques, like EBSD and synchrotron [87]. Prior to using such experimental techniques, we first wanted to check whether texture gradients induced by the interface may have been missed by the foregoing measurements. In Figs. 10d, 11d, we examine the textures predicted for only those Zr and Nb grains joined to the Zr/Nb interface. As shown, the textures possess the same peak components, suggesting that no pronounced texture gradient developed.

Taken together, these results indicate that bulk texture development in the polycrystalline layers is 1) not greatly affected by the interface, 2) even in the nanoscale composite, is primarily a consequence of dislocation slip, and 3) deformation twinning was not a predominant mechanism.

5.5 Model predictions of slip activity

We used the model to predict the active slip modes underlying texture evolution. Figure 13 shows the relative slip activity in the polycrystals as a function of strain. The slip activities in single-phase Zr and Nb are the same as those in the Zr and Nb phases within the composite. For Zr, we find that within the first 0.3 strain, the deformation is accommodated by pyramidal slip and prismatic slip. However, at larger strain, basal slip becomes active and pyramidal slip even less so. It is important to note that the substantial amount of basal slip (25%) is considered anomalous and appears to arise in the event of large strain deformation. Similar large strain studies on pure Zr predicted an unexpected amount of basal slip [24, 60, 61]. It was further revealed in [24] that anomalous basal slip does not arise because the physical barriers for basal dislocation glide have been reduced but easy prismatic $\{a\}$ slip has sufficiently strain-hardened and the crystallographic texture has evolved in large-strain deformation such that basal slip becomes relatively favorable. For the Nb phase, $\{110\}$ slip and $\{112\}$ slip are both active, with the former being predominant. The ratio of the two slip activities does not change after a strain of 1.1.
6. Conclusions

In this work, we present a combined dislocation density-crystal plasticity finite element model (DD-CPFE). Unlike mean-field techniques, this DD-CPFE model can provide spatially resolved fields of displacement, stress, strain, and grain reorientation both within the grains and near boundaries and interfaces and can capture the effects of grain-grain and interface-grain interactions. It is also designed to treat large strain deformation by a method of repeated deformation steps and passing key state variables.

We use this new model to predict texture evolution and active deformation mechanisms in a two-phase hcp Zr/bcc Nb lamellar composite during a severe plastic deformation (SPD) technique called accumulative roll bonding (ARB). We find that the calculated textures of each phase in the composite are the same as those of each phase rolled alone. The model also finds that texture gradients do not develop across the layer thickness. Notably, the predicted textures themselves and the similarity between the composite and monolithic textures are in reasonable agreement with experimental observation on micron- to nano-scale layered Zr/Nb ARB composites [1].

The model indicates that for Zr, in the later stages of deformation, prismatic slip is predominant, and secondly pyramidal and basal slip. The amount of basal slip is unusually large (25%), consistent with other reports of Zr in large-strain deformation. In the Nb phase,
{110} < 111 > and {112} < 111 > slip are both active, with the former providing more accommodation.

The consistency between the model and measurement for both the micron-SPD bimetal and the nano-SPD bimetal suggests that 1) neither the nanoscale grain sizes nor the bimetal Zr/Nb interfaces induce deformation mechanisms different from those at the coarse-grain scale, and 2) dislocation-mediated plasticity accommodates deformation at all scales from 100 µm to 0.1 µm. This is remarkable contrast to ARB Cu-Nb composites, showing yet another interesting difference between cubic and hcp metals that arises in the SPD and nano-scale regimes.

The DD-CPFE model used here does not account for any possible modification of the constitutive model by the interface. The influence of grain boundaries and interfaces in plasticity (dislocation nucleation and transmission) is an intense field of research [10, 88], but the current understanding of hcp/bcc interfaces is not sufficient for developing an interface-modified constitutive model for the present work. The multi-scale model presented here is sufficiently physically based that such a modification can be implemented later without changing the basic framework.

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