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Anomalous Basal Slip Activity in Zirconium under High-strain Deformation

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In this letter, we reveal anomalous basal slip activity in zirconium under high strains. The frequently reported classical rolling texture of Zr is shown to develop as a result of substantial amounts of basal slip. The reason is not that physical barriers to basal slip have become easier but that over a large straining period, easy prismatic $\langle a \rangle$ slip has significantly strain-hardened and crystallographic texture has evolved to be more favorable for basal slip. Basal slip is, therefore, an important deformation mechanism in Zr at room temperature under high to severe strain-deformation conditions.

Keywords: Hexagonal Metals, Zirconium, Deformation Mechanisms, Basal Slip, Accumulative Roll Bonding

Deformation to high strains is still an unexplored region of material response, involving unexpected deformation mechanisms. A case as familiar as the formation of the classical rolling texture of zirconium (Zr) has proven to be one such example. The formation of this texture to saturation requires large strains (>2.0) and how it develops over such an extended, severe strain period has yet to be clarified. Remarkably, experimental reports of the saturated rolled texture of Zr [1–6] are consistent, albeit for higher-order texture variations, despite differences in alloy content, rolling temperatures, initial grain size and initial texture. Thus, the explanation for its development needs to be universal, involving a fundamental phenomenon that operates in all cases.

We show that the classical Zr rolling texture requires substantial basal slip activity, which challenges conventional knowledge in deformation behavior of Zr. A large number of experimental and theoretical studies performed on single-crystal [7–11] and polycrystalline [12–16] Zr and its alloys established that slip along the $\langle 11\bar{2}0 \rangle$ ($\langle a \rangle$) directions occurs primarily on the prismatic $\{1\bar{1}00\}$ planes and not the basal $\{0001\}$ planes. Thus, while basal slip systems are the easy glide systems

in many hexagonal close-packed (hcp) metals with a c/a ratio near 1.633, such as magnesium [17–19] and beryllium, [20–23] it is not regarded as the prevalent mechanism in metals with a c/a ratio above 1.633 such as Ti [24,25] and Zr, [12,26,27] particularly during room-temperature deformation. The former materials show a strong basal texture aligned with the sample normal direction (ND), while the latter materials show splitting along the transverse direction (TD). We show that this splitting develops not only because of expected prismatic slip but also because basal slip becomes prevalent at high strain levels. The activity of basal slip and issues in predicting texture for various hexagonal metals under severe plastic deformation (SPD) have been discussed in [28,29]. In Zr, local activation of basal slip near twins and kink bands, [12] cracks [26,30] and free surfaces [26,27,31,32] could be expected, but substantial amounts of basal slip would be considered anomalous. The distinction between such localized occurrences vs. extensive participation in accommodating imposed plastic strain can be assessed by examining crystallographic texture evolution in the material during deformation. While the former examples of localized basal slip would have a negligible effect on

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bulk texture evolution, the latter case of prevalent activity in the plasticity of a material would induce a profound, readily measurable effect.

In this work, we compare predicted and measured texture to support our hypothesis. If ample basal slip occurs in Zr during rolling then there must be clear signatures in the experimental textures. The three types of dislocations considered here (prismatic $\langle a \rangle$, basal $\langle a \rangle$ and pyramidal $\langle c + a \rangle$ slip) glide on different independently oriented planes in the hcp crystal and do not have the same impact on texture evolution. Consequently, successful prediction of crystallographic texture evolution is not possible unless the active slip planes and directions (relative activities) were predicted accurately. In this regard, theoretical analysis of texture evolution, particularly over large strain deformation, provides a more rigorous indicator of basal slip activity than the evolution of flow stress or grain morphology alone.

Here, the model utilized for texture and slip activity predictions contains at its core a physically based dislocation density model for dislocation glide and storage on individual slip systems. We carry out simulations that begin with the measured initial texture, which is different from that of rolling, and deform the material to texture saturation at high strains. The main conclusion of this work is that the classical rolling texture of Zr results from copious amounts of basal slip. Basal $\langle a \rangle$ slip activates after a deformation strain of approximately 0.5 and eventually attains a substantial relative slip activity of approximately 25%. For each type of slip dislocation, we characterize its Peierls stress, activation enthalpy for thermally activated de-pinning from obstacles (de-pinning potential), drag stress and storage rate coefficients. We find that prismatic and pyramidal slip systems possess substantially lower Peierls stresses than basal slip. With this, we conclude that the cause for basal slip to operate to such an extent

is that easy prismatic $\langle a \rangle$ slip has strain-hardened and crystallographic texture has evolved such that basal $\langle a \rangle$ slip becomes favorable. Thus, this anomaly is a consequence of large strain deformation and accordingly is responsible for Zr behavior in high-strain-deformation conditions.

The material used in this study is high-purity zirconium with the following chemistry expressed in weight parts per million (Wt. ppm) Hf = 35, Fe < 50, Al < 20, V < 50, O < 50, N < 20, C < 22 and Zr balance.[33] The material was initially upset forged, subsequently clock rolled and annealed at 550°C for 1 h. This produced a strongly textured plate, whose normal is nearly aligned with the c -axis. Finally, the material has undergone further straight rolling of ~60% reduction and annealing at 600°C for 1 h. The resulting microstructure and texture are shown in Figure 1, which is the starting material in our study. The material exhibits equiaxed, twin-free grains with an average grain size of about 40 μm and strong basal texture slightly tilted toward the TD.

High-strain rolling deformation was achieved by a SPD technique called accumulative roll bonding.[5,34] This technique was used to produce a multilayered Zr and Nb composite used in this study to investigate the texture evolution of the Zr phase. The annealed zirconium plate and annealed Nb plate were ultrasonically cleaned in a bath of acetone and wire-brushed in preparation for bonding. The plates of material were then stacked and roll-bonded together at room temperature using a single high-strain rolling pass of ~50% reduction. The bonded material was cut in half and the process of surface cleaning, stacking and roll bonding was iterated in order to produce samples having experienced various amounts of cumulative strain. As an example we show the resulting layered composite deformed to a strain of 2.5 with corresponding layer thicknesses of approximately 20 μm in Figure 2(a). Figure 2 also shows the textures

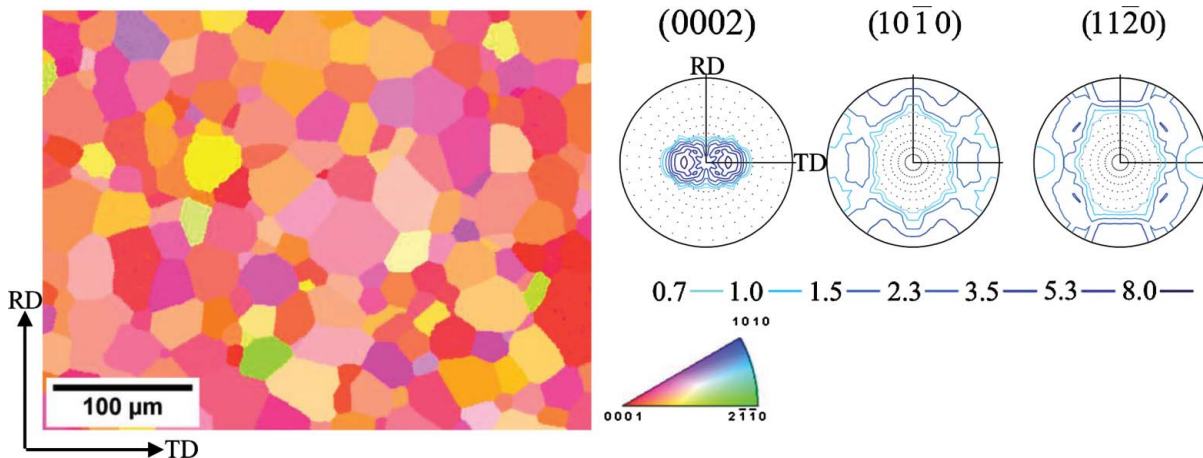


Figure 1. EBSD orientation map and pole figures showing initial microstructure and texture in the as-annealed sample of rolled zirconium. The colors in the orientation maps indicate the orientation of the ND sample direction with respect to the grain orientations.

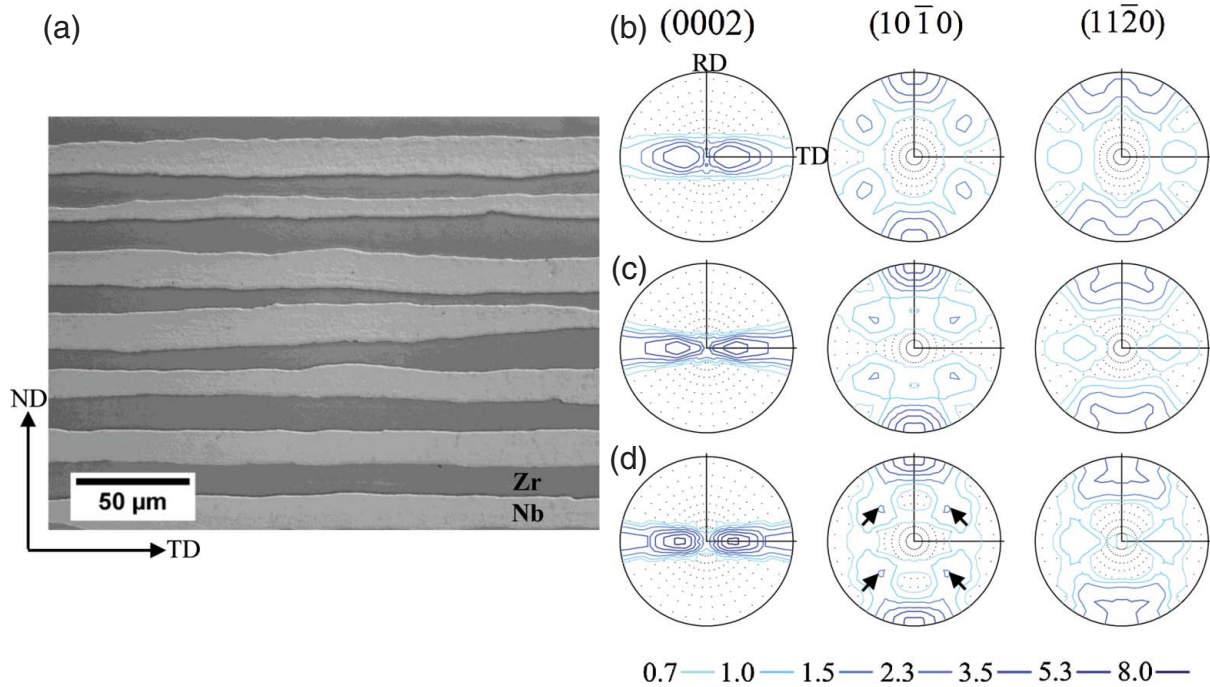


Figure 2. (a) SEM micrograph of a Zr-Nb composite processed by ARB to a strain of 2.5. Measured pole figures showing texture in the zirconium phase processed by ARB to strains levels of (a) $\varepsilon \approx 2.0$, (b) $\varepsilon \approx 2.5$ and (c) $\varepsilon \approx 3.5$. The EBSD scans were approximately positioned in the middle of an inner zirconium layer in the RD-ND plane. The texture appears to have saturated by a strain of 2.0.

measured by electron backscattered diffraction (EBSD) at different levels of rolling strain of approximately 2.0, 2.5 and 3.5. At large strains, a lot of measurement points were purely indexed. For plotting textures we used only measurements with a confidence index of 0.3 or greater.

These measurements indicate that the main rolling texture components are defined at large strains on the order of 2.0 or more. Dominant texture components are consistent with reports in many prior studies.[1–6] During rolling the strong and slightly tilted (0002) texture component in the ND has spread toward the TD direction along the ND-rolling direction (RD) plane with concentration 30–50° from the ND direction. The (10 $\bar{1}$ 0) components tend to align with the RD and concentrate away from the TD and the RD directions for about 30° and 60°, respectively (see arrows). The (11 $\bar{2}$ 0) pole exhibits a spread of intensities toward the RD direction from the ND-TD plane and a peak concentrated 50° toward the TD direction along the ND-RD plane.

We employ a dislocation density single crystal (SX) model, which defines a dislocation density ρ for each slip mode α (e.g. prismatic, pyramidal) as a state variable and evolves each with strain according to thermally activated glide motion. The SX model is then utilized to govern dislocation activity within individual grains of a polycrystalline aggregate. The relationship between grain and polycrystal deformation in rolling is modeled using a polycrystal visco-plastic self-consistent framework,

[e.g. 25,35–38], which provides the final prediction of texture.

The SX model has its roots in the thermodynamic theory of plastic slip, described by glide of arrays of dislocations interacting with other groups of dislocations in a network. When dislocation arrays glide in a deforming crystal, they encounter obstacles, such as other dislocations, that can potentially pin them. In this theory, the rate at which dislocations glide is controlled by the rate at which they can de-pin from these sites via a combination of thermal activation and mechanical stress (the resolved shear stress). The rate regime where such kinetics best applies is that which lies above the creep regime (10^{-5} /s), but below that of linear drag (10^6 /s).

Dislocations in the crystal that serve as obstacles are categorized as those belonging to the density of random forest $\rho_{\text{for}}^{\alpha}$ dislocations or dislocations organized into patterns $\rho_{\text{sub}}^{\alpha}$ (substructure). For a given slip mode α , the resistance to glide is a sum of a Peierls stress τ_0^{α} , and forest and substructure interaction stresses $\tau_{\text{for}}^{\alpha}$ and $\tau_{\text{sub}}^{\alpha}$, i.e.

$$\tau_c^{\alpha} = \tau_0^{\alpha} + \tau_{\text{for}}^{\alpha} + \tau_{\text{sub}}^{\alpha}. \quad (1)$$

As $\rho_{\text{for}}^{\alpha}$ and $\rho_{\text{sub}}^{\alpha}$ increase, the interaction distances between dislocations decreases, increasing the physical barriers to dislocation glide. This is found to yield the following relation between the stresses $\tau_{\text{for}}^{\alpha}$ and $\tau_{\text{sub}}^{\alpha}$ and

the dislocation densities ρ_{for}^α and ρ_{sub} [37,39]:

$$\begin{aligned}\tau_{\text{for}}^\alpha &= \chi b^\alpha \mu^\alpha \sqrt{\rho_{\text{for}}^\alpha} \quad \text{and} \\ \tau_{\text{sub}}^\alpha &= k_{\text{sub}} \mu^\alpha b^\alpha \sqrt{\rho_{\text{sub}}} \log \left(\frac{1}{b^\alpha \sqrt{\rho_{\text{sub}}}} \right),\end{aligned}\quad (2)$$

where $\chi = 0.9$ is a dislocation interaction parameter and, μ^α is the shear modulus and $k_{\text{sub}} = 0.086$ is a mathematical parameter that recovers the Taylor law for low dislocation densities.[40] Note that τ_{sub}^α takes into account latent hardening effects between slip systems implicitly through the development of substructure within the grain due to imperfect recovery reactions in all slip systems. The evolution of the stored forest density ρ_{for}^α is governed by competition between the rate of storage and the rate of dynamic recovery:

$$\begin{aligned}\frac{\partial \rho_{\text{for}}^\alpha}{\partial \gamma^\alpha} &= \frac{\partial \rho_{\text{gen, for}}^\alpha}{\partial \gamma^\alpha} - \frac{\partial \rho_{\text{rem, for}}^\alpha}{\partial \gamma^\alpha} = k_1^\alpha \sqrt{\rho_{\text{for}}^\alpha} - k_2^\alpha (\dot{\epsilon}, T) \rho_{\text{for}}^\alpha, \\ \Delta \rho_{\text{for}}^\alpha &= \frac{\partial \rho_{\text{for}}^\alpha}{\partial \gamma^\alpha} |\Delta \gamma^\alpha|,\end{aligned}\quad (3)$$

where k_1^α is the rate coefficient for dislocation storage by statistical trapping of gliding dislocations by the forest network and k_2^α is the rate coefficient for dynamic recovery,[37] which is given by

$$\frac{k_2^\alpha}{k_1^\alpha} = \frac{\chi b^\alpha}{g^\alpha} \left(1 - \frac{kT}{D^\alpha b^3} \ln \left(\frac{\dot{\epsilon}}{\dot{\epsilon}_o} \right) \right). \quad (4)$$

In Equation (4), k , $\dot{\epsilon}_o$, g^α and D^α are the Boltzmann constant, a reference strain rate, effective activation energy and a drag stress, respectively. Dynamic recovery relies on several possible dislocation maneuvers, such as dislocation cross slip and climb, to overcome obstacles, and the activation barrier g^α is associated with that of the dominant one of all such de-pinning processes, which is an obvious simplification of an otherwise complex statistical problem. These same recovery processes lead to the formation of dislocation substructures and as a consequence, the rate of substructure development is coupled to the rate of dynamic recovery of all active dislocations through:

$$\Delta \rho_{\text{sub}} = \sum_\alpha q^\alpha b^\alpha \frac{\partial \rho_{\text{rem, for}}^\alpha}{\partial \gamma^\alpha} |\Delta \gamma^\alpha|, \quad (5)$$

where q is a dislocation recovery rate coefficient defining the fraction of α -type dislocations that do not annihilate but become substructure. Quantities with superscript α signify the slip mode. Prismatic, pyramidal and basal slip dislocations have different atomic core structures [41,42] and they in principle should have their own Peierls stress, activation barrier for de-pinning, drag stress and trapping rates.

Table 1. Constitutive parameters for evolution of slip resistance.

α	$\alpha = 1$, prism slip	$\alpha = 2$, basal slip	$\alpha = 3$, pyramidal slip
τ_0^α [Mpa]	20.0	700.0	160.0
k_1^α [m ⁻¹]	1.25×10^8	1.25×10^{10}	2.25×10^8
g^α	3.75×10^{-3}	3.675×10^{-2}	6.5×10^{-2}
D^α [Mpa]	3.3×10^2	3.3×10^2	1.0×10^2

With the current model formulation, it has been shown previously that texture evolution in polycrystalline Zr deformed up to moderate strain levels and over a wide range of temperatures (from liquid nitrogen to above room temperature) can be predicted with prismatic slip as the easiest deformation mode, pyramidal slip as the relatively hard deformation mode and the most commonly observed twinning modes $\{10\bar{1}2\}\langle 10\bar{1}1 \rangle$ and $\{11\bar{2}2\}\langle 11\bar{2}3 \rangle$. [14,37,43] In addition, it has proven reliable and robust in predicting the behavior of Zr when loaded in multiple directions [37] and in temperature jump tests and strain path changes.[13] The parameters for prismatic $\langle a \rangle$ and pyramidal $\langle c + a \rangle$ slip are given in Table 1. While in all these cases, basal slip was not required, the typical strain level only ranged from 0.1 to 0.3. Thus, to maintain congruence with the main deformation mechanisms established by these prior works, as well as several other experimental observations and other modeling efforts,[13,37,44] the same model that finds basal slip active at severe strains should also find that basal slip is not prevalent at small to moderate ones. The starting values of the hardening parameters for prismatic and pyramidal slip were taken from an earlier study.[37] The parameters for basal slip are characterized here based on the texture data.

Starting with the initial measured texture represented by 15,000 orientations in Figure 1, we carried out simulations of rolling to high strains sufficient to achieve saturation. Figure 3 shows the predicted saturated texture using the original model with prismatic $\{1\bar{1}00\}\langle 11\bar{2}0 \rangle$ slip, pyramidal $\{10\bar{1}1\}\langle \bar{1}\bar{1}23 \rangle$ slip, $\{10\bar{1}2\}\langle 10\bar{1}1 \rangle$ twinning and $\{11\bar{2}2\}\langle 11\bar{2}3 \rangle$ twinning made available. The corresponding variation in slip activity with strain shown in Figure 3 indicates that this texture developed by activating prismatic and pyramidal slip only. The relative slip activity per mode is defined as a contribution to shear of the mode normalized by the total contribution of all slip modes. The lack of twinning can be explained by the room-temperature deformation, the orientation of the initial texture with respect to the rolling and the high nucleation stress for the $\{11\bar{2}2\}\langle 11\bar{2}3 \rangle$ contraction twin in Zr. It can be seen that these predictions severely disagree with the experimental measurements in Figure 2. We hypothesize that this discrepancy results from a lack

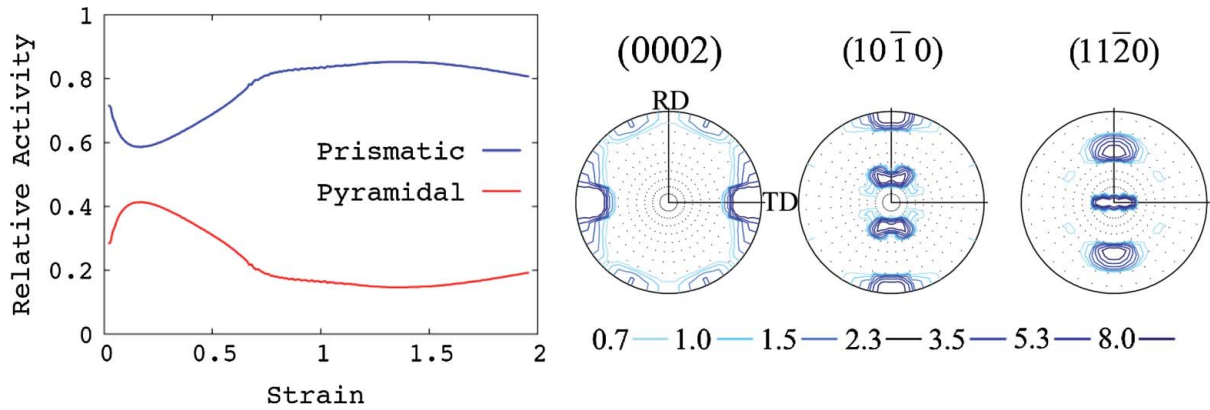


Figure 3. Predicted relative activities of prismatic and pyramidal deformation modes contributing to plasticity during plane-strain-compression of zirconium. Pole figures showing simulated texture in zirconium under plane-strain-compression conditions at a strain of 2.0. The simulations were performed using the VPSC model with constitutive parameters for zirconium reported in [37].

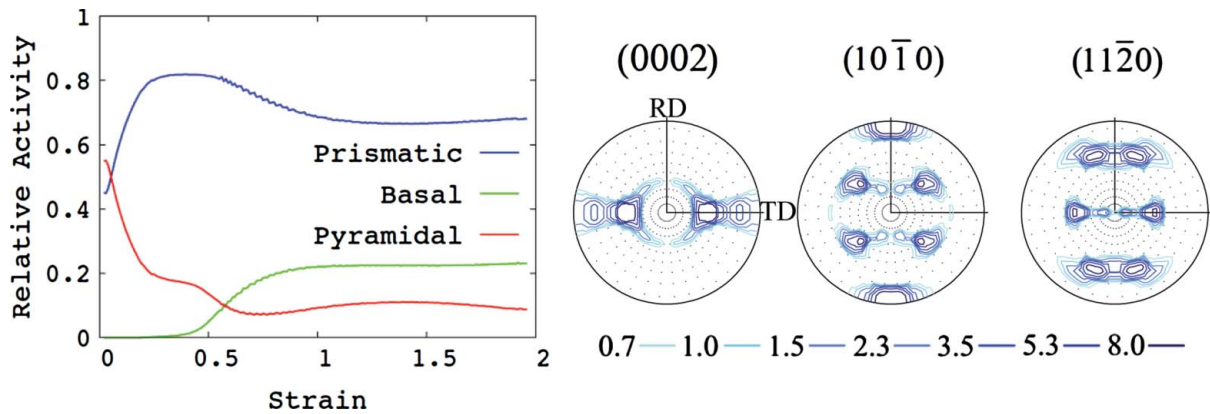


Figure 4. Predicted relative activities of prismatic, basal and pyramidal deformation modes contributing to plasticity during plane-strain-compression of zirconium. Pole figures showing simulated texture in zirconium under plane-strain-compression conditions at a strain of 2.0. The simulations were performed using the VPSC model reported in [37] with constitutive parameters estimated in this study.

of extensive basal slip, which becomes favorable when the initially easy prismatic slip and secondary pyramidal slip strain-hardened in large strain deformation.

While keeping the kinetics model in Equations (3)–(5) for prismatic and pyramidal the same, we integrated the same model for basal slip (Table 1). For basal slip we obtain a much higher Peierls barrier (5–10 times), trapping coefficient (two orders of magnitude) and activation barrier (one order of magnitude) than those for prismatic. Interestingly the drag stress for prismatic and basal slip dislocations, which share the same Burgers vector, was estimated to be the same.

Figure 4 shows the saturated rolling textures predicted by the model when basal slip is also made available. Basal slip has noticeably altered texture evolution in rolling and enabled achievement of the main texture features consistent with experimental observation. The calculated texture contains the tilted (0002) texture component from the ND direction and the spread of the (0002) poles toward the TD direction along ND-RD plane. From the (10 $\bar{1}$ 0) pole figure, we observe the characteristic

alignment of the (10 $\bar{1}$ 0) poles with the RD and formation of maxima at about 60° and 30° from the RD and the TD directions, respectively. The predicted (11 $\bar{2}$ 0) pole figure captures the six main peaks observed experimentally.

Since we employ a characteristic basal dislocation density law, one that is separate from the prismatic or pyramidal dislocation density law, and use these three laws to govern slip activation within individual grains in a polycrystal, we can predict (1) when and where basal slip activates, (2) instantaneously at all strains, the fraction of the deformation it accommodates relative to prismatic and pyramidal slip and (3) evolution of dislocation density and slip resistance. In Figure 4, we analyze the contribution of basal slip at all strains in texture development by plotting the predicted relative activities of prismatic, basal and pyramidal slip. The predictions show that for the initial period of straining, prismatic and pyramidal slip are activated, but at a strain of 0.5, we observe the onset of basal slip. With further straining, basal slip attains a non-negligible relative activity of 25%, higher than pyramidal slip. Neither twinning mode was

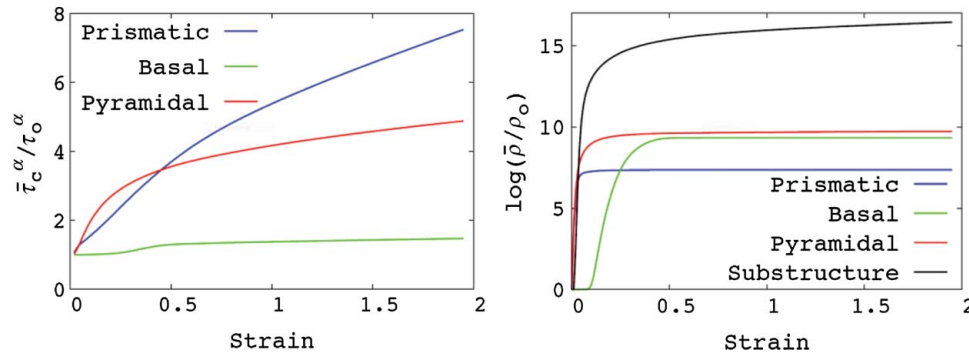


Figure 5. (a) Evolution of prismatic, basal and pyramidal slip resistances when averaged over the entire polycrystal. (b) Evolution of the average forest dislocation density for prismatic, basal and pyramidal slip modes and average substructure dislocation density. The slip resistances as well as the dislocation densities were normalized by their respective initial values. The dislocation substructure in (b) mainly is comprised of prismatic dislocations.

activated. Correlating this result with texture evolution, we find that basal slip is responsible for concentrating the basal poles $30\text{--}50^\circ$ from the ND direction in the ND-TD plane. Figure 5(a) compares the corresponding evolution of slip resistance for the three slip modes normalized by the respective Peierls stresses. The predicted dislocation density evolution is given in Figure 5(b). These calculations reveal that while prismatic slip retains the lowest slip resistance and remains the dominant slip mode over the entire strain interval, accumulation of prismatic glide dislocations with strain causes its slip resistance to experience the largest percentage increase at strains of 0.5 and higher. This enhancement promotes alternative $\langle a \rangle$ slip, such as basal slip, in favorably oriented crystals. The dislocation density predictions in Figure 5(b) indicate that although the onset of basal slip is delayed and its activity is not dominant, the stored forest dislocation network at 1.0 strain and beyond still contains a substantial amount of basal slip dislocations.

It is noteworthy that the pronounced contribution of basal slip to rolling deformation occurred despite a much higher Peierls barrier and hardening rates (higher trapping and lower recovery) than either prismatic or pyramidal slip (Table 1). Evidently, at sufficiently large strains, basal slip becomes active due to the combined effect of strain hardening of the usually easy prismatic slip and attainment of suitable crystal orientations.

Earlier studies have also suggested that basal slip is a possible secondary system when deforming Zr, for instance in rolling,[6] compression at room temperature to strains of -0.8 , [45] channel die compression at room temperature to strains of -0.4 , [31,32,46] equal-channel angular extrusion (ECAE) at elevated temperatures [47,48] and room temperature.[49] In another polycrystal modeling study, matching the evolution of lattice strain measurements obtained in situ by neutron diffraction measurements in Zircaloy-2 required considering the onset of basal slip.[50] These studies, however, have not been able to reliably determine its contribution in

large strain deformation compared with other potentially active secondary systems, such as pyramidal $\langle c + a \rangle$ slip and deformation twinning. Prior polycrystal modeling simulations utilized either constant (non-evolving) slip-resistance values [35,45] or slip-resistance values whose ratio changed (decreasing activity of certain systems, increasing of others) without a hardening law [6] or using a phenomenological function,[46] began with sharp textures that corresponded to or were already close to that for rolling, and imposed moderate deformation. With these prior approaches, the contribution of basal slip activity could not be determined. First, the reported slip-resistance parameters would not apply to both small and large strain or be unique. For instance, in one case, basal and pyramidal slip had the same constant slip resistance [46] and in another basal slip had a much lower slip resistance than pyramidal slip [6,45]; neither combination is guaranteed to lead to slip activity appropriate at other deformation levels or conditions. Second, they report different deformation mechanisms. Some models predicted primarily prismatic and basal slip activity,[6,45] others prismatic slip and pyramidal,[46] and yet others prismatic slip and twinning.[16,35] One exception is that of the modeling work of Yapici et al. [49], which showed that the texture after 1.0 simple shear by ECAE results from the onset of basal slip activity after 0.3 strain, even when they set an initial slip resistance for basal slip higher than that of pyramidal or prismatic slip.

Experimentally it is difficult to observe basal slip in action or to quantify its slip activity. Most techniques, which have reported basal slip, are local measurements, such as slip trace surface analysis or transmission electron microscopy (TEM). Although the results from single-crystal tests of Zr may have less ambiguity, they do not embody the important effect that a collection of interacting grains and texture can have on intra-grain slip activity. The slip activity within individual grains of Zircaloy-2 deformed in tension to a strain of 0.15 can be studied by combining line profile analysis of micro-diffraction X-ray

measurements from synchrotron radiation with electron backscatter diffraction.[51] However to date, the technique requires grains to be at least 30 μm , which can be too large compared with the usually refined grains in severely deformed materials.

In this letter, we have shown the first conclusive evidence based on a physically based model that the classical Zr rolled texture is achieved by substantial basal slip activity. The amount of basal slip, being well over 25%, is anomalous. We reveal that the reason is not because the physical barriers for basal slip dislocation glide have been reduced but that under high-strain deformation, easy prismatic $\langle a \rangle$ slip has significantly strain-hardened and the crystallographic texture has evolved to a more favorable orientation for basal slip.

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