Exceptional Friction Mitigation via Subsurface Plastic Shear in Defective Nanocrystalline Ceramics

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Single-crystal and microcrystalline ceramics classically fail via brittle fracture under loading. Here, we report that atomic layer deposition {0002}-textured ZnO films, with nanocolumnar grains and defective sub-stoichiometric structure, exhibit nanocrystalline plasticity and exceptionally low sliding friction and wear. These films were tailored to contain low-energy basal stacking fault planes parallel to the film surface. Cross-sectional high-resolution TEM studies inside friction-induced surfaces coupled with density functional theory calculations revealed the fundamental mechanism of this unexpected behavior. We show that sliding on {0002}-textured nanocrystalline ZnO films increases partial dislocation density through intrafilm shear, via glide of partial dislocations, on {0002}-stacking fault planes.

Keywords: Nanocrystalline Ceramics, Friction, Dislocations, Plastic Deformation, Density Functional Theory

Friction and the attendant wear of materials is a millennia old and, yet, a persistent problem, causing reduced efficiencies of engines, turbines, industrial machinery, and other technologies.[1] Friction arises whenever one material slides over another and is commonly measured macroscopically by the friction coefficient $\mu$. Third bodies, such as liquid lubricants, atomically thin surfaces, and/or chemically and structurally altered wear surfaces, influence friction.[1–3] While entrapped in the moving interface, they often go unnoticed because they are buried in the contact. Nonetheless, they influence how materials accommodate the relative sliding motion, known as velocity accommodation modes (VAM), with interfacial sliding between the third body and the wearing surface being the most common.[3] The friction coefficient is controlled by a velocity accommodation parameter, often referred to as the interfacial shear strength, $\tau_0$, where $\tau_0 = \mu P$ and $P$ is the contact pressure. This shear strength is related to, but not necessarily the same as, the shear strength of the material or third body. Godet [2] postulated the existence of other VAM, each with its own friction process. However, many of these have not been experimentally observed due to the lack of appropriate in situ triboscopy techniques or their occurrence in the subsurface.

Traditional liquid lubricants fail under extreme temperature, oxidative, and stress environments due to diminished intrinsic interplanar mechanical sliding. Therefore, the recent focus is to develop a new class of solid lubricants for use in extreme environments.[4] Nanocrystalline (NC) ZnO with a hexagonal wurtzite crystal structure is a promising candidate due to its low-friction deformation behavior.[4] This expectation is supported by theoretical [5] and computational [6–8] studies that show a change in deformation mechanisms from traditional dislocation-mediated slip to grain boundary sliding and rotation in randomly oriented NC ceramics with grains below 30 nm.

In this letter, we couple density functional theory (DFT) calculations, friction experiments, site-selective focused ion beam (FIB) microscopy, and cross-sectional high-resolution transmission electron microscopy (HRTEM) to probe friction-induced, buried subsurfaces in textured NC ZnO. We have identified a novel subsurface intrafilm shear VAM mechanism that significantly reduces friction and increases ductility. This mechanism is not found in either single-crystal or microcrystalline ZnO. We contend that the subsurface intrafilm shear mechanism can operate in other textured NC ceramics and could dramatically expand the
set of lubricious materials available for use in extreme environments.

Single-crystal and microcrystalline ceramic oxides are inherently brittle, which results in cracking and subsequently increased abrasive frictional losses. NC ceramic oxides, in contrast, exhibit improved mechanical and tribological properties.[4,6–9,11] For instance, the friction coefficient of NC ZnO (μ = 0.1–0.2) is significantly less than hot-pressed randomly orientated microcrystalline ZnO (μ = 0.7). This is achieved by controlling the ZnO (0002)-textured grain structure and oxygen sub-stoichiometry.[4] This low friction was proposed to be due to the defective (0002)-nanocolumnar grain structure with subgrains that can accommodate plastic deformation.[4] Those authors suggested that site-selective TEM studies inside the worn subsurface are needed to conclusively determine the friction dissipation mechanisms. In this letter, we report the first results of such a characterization.

ZnO [12–14] and other hexagonal wurtzite crystals [15,16] are known to develop a high density of stacking faults (SFs) in combination with threading and partial dislocations (PDs) during film deposition. We hypothesize that these growth defects force dislocations to glide parallel to the interfacial sliding direction to accommodate shear. Interrogation of NC ZnO defect structure before and after sliding by TEM coupled with DFT calculations of the formation energies of these SFs is used to elucidate the fundamental plasticity mechanisms.

Atomic layer deposition (ALD) nanolaminate tri-layer stacks of ZnO (~100 nm thick)/Al2O3 (~20 nm)/ZrO2 (~100 nm) were grown on Si (100) substrates as described elsewhere.[17] The amorphous Al2O3 below the ZnO layer helps the low surface energy (0002) plane of ZnO to grow with the c-axis preferred orientation by suppressing other competing higher surface energy planes, e.g. (1 0 1 0) and (1 0 1 1).[11] The underlying tetragonal ZrO2 acts as a load-bearing layer (at moderate contact pressures of ~1 GPa) to minimize subsurface frictional shear stresses. The deposited nanolaminate was first annealed in vacuum at 400°C for 2 h to determine changes to defect structures (SFs and PDs) and friction. Previous X-ray diffraction (XRD) and cross-sectional HRTEM analyses confirmed that the as-deposited nanolaminates possess nanocolumnar ZnO grains of 28 nm average width and with random rotational orientation.[11,18] Annealing promoted limited grain growth to 34 nm as seen by XRD peak narrowing. The absence of XRD peak shifts in both the as-deposited and annealed nanolaminates indicates negligible lattice strain. Furthermore, the ZnO (0002)-orientated grains have a texture coefficient (TC) of 2.9 determined using the Harris method, where a TC > 1 indicates preferential orientation. X-ray photoelectron spectroscopy (XPS) revealed that the as-deposited Zn0.51O0.49 layer became more sub-stoichiometric (Zn0.53O0.46) with annealing. This has been linked to condensation of oxygen vacancies introducing a missing or extra ZnO (0002)-lattice plane and incoherent boundaries between adjacent nanocolumnar grains.[19] These are sources of ZnO growth basal stacking faults (BSF) and their crucial role in mitigating friction is discussed later.

Unidirectional sliding friction tests were conducted at room temperature in open air (~40% RH) using a stationary 1.59 mm diameter Si3N4 ball as a counterface material. Normal loads (L) of 0.245, 0.49, 0.98, and 2.45 N were applied, which correspond to initial mean Hertzian contact pressures of 0.46, 0.58, 0.72, and 0.98 GPa, respectively. The sliding velocity was 2.1 cm/s and at least five tests were performed for each condition. A transducer in the load arm measured the tangential load (F) over a sliding distance of 200 m. The friction coefficient μ is F/L and is in steady state when it changes by less than 5% from cycle to cycle. Wear rates (in mm3/N m) were also determined as the wear surface volume divided by the normal load and by the total distance traveled by the Si3N4 counterface. It was computed by multiplying the averaged cross-sectional area of the wear track, measured by surface profilometry traces, by the circumference of the wear track (assuming uniform wear) and dividing the result by the normal load and by the total distance. In addition to the nanolaminates, monolithic (0001) ZnO single crystal (SC) (oxygen surface terminated, MTI Corp, Richmond, CA, USA) and ZnO with randomly orientated NC surface grains (Cerac Inc, Mayfield Heights, OH, USA) were tested under 0.72 GPa contact pressure.

The steady-state friction coefficients μss of textured NC ZnO shown in Figure 1(a) were fitted to a power law equation of the normal load. The fits of μss = L−0.32 and μss = L−0.28 for as-deposited and annealed ZnO, respectively, agree well with the Hertzian contact model, where τ0 is the interfacial shear strength between the sliding surfaces, R is the ball radius, and E* is the composite elastic modulus of the materials. The term α represents the pressure dependence of shear strength—it is the lowest attainable friction coefficient for the testing couples. Figure 1(a) shows that μss values for both as-deposited and annealed NC ZnO layers decrease with increasing L (or decreasing inverse mean Hertzian contact pressure, P H). This friction behavior contrasts Amonton’s first law of friction wherein μ is independent of L. Similar non-Amontonian friction behavior was seen in molecular dynamic friction simulations of NC SiC sliding on diamond.[20] The linear relationship between μ and L−1/3 in Equation (1) has been experimentally verified for a number of low-friction solid lubricant coatings.[21]
The steady-state friction coefficients $\mu_{ss}$ of SC ZnO and NC-randomly oriented ZnO grains plotted in Figure 1(a), in contrast, are significantly higher than the NC-textured ZnO grains. This suggests that texturing of (0002) grains plays an important role in reducing interfacial shear strength as opposed to just having NC-sized grains. Also, a favorable SC (0001)-basal plane orientation in ZnO by itself does not yield low friction, alluding to the importance of a high density of grain boundaries. These results also substantiate the sensitivity of the macroscopic friction measurements in differentiating between NC-textured and randomly orientated ZnO grains. Another important observation is that the annealed ZnO layer exhibited lower friction than the as-deposited layer at each corresponding contact pressure. Therefore, mechanistic studies are needed to explain these experimental results. Specifically, the exact crystal defect structure dependence of deformation mechanisms needs to be identified using advanced microscopy inside the deformed surfaces and subsurfaces, and this has been done below.

Ramping of the normal load during sliding also allows us to explore the pressure dependence of $\mu_{ss}$ on the interfacial shear strength via the equation

$$\mu_{ss} = \frac{F}{L} = \frac{A_R \tau}{L} = \frac{\tau}{P_H} = \frac{\tau_o}{P_H} + \alpha,$$

where $A_R$ is the real contact area according to Bowden and Tabor.\[22\] Fitting the $\mu_{ss}$ values in Figure 1(a) as a function of $P_H$ yields mean $\tau_o$ (and $\alpha$) values of 151 (0.021) and 98 (0.013) MPa for the as-deposited and annealed NC ZnO nanolaminates, respectively. These values are comparable to many low-friction solid lubricant films.\[21\] Note that the normal load dependency on the friction coefficient (Equation (1)) and the pressure-induced shear stress (Equation (2)) analyses for NC ZnO are valid because our cross-sectional HRTEM analysis shows that underlying Al$_2$O$_3$ and ZrO$_2$ nanolaminates and the Si substrate do not plastically deform.

In addition to friction coefficients, the resulting sliding wear rates are another important property. The wear rates at a normal load of 0.98 N (0.72 GPa contact pressure) are $2 \pm 0.8 \times 10^{-7}$ mm$^3$/N m and $8 \pm 2 \times 10^{-8}$ mm$^3$/N m for as-deposited and annealed NC-textured ZnO grains, respectively. The slightly lower wear rate with annealing is in good agreement with the trend in friction coefficients in Figure 1. In contrast, both the NC-randomly oriented ZnO grains and SC (0001) ZnO wear rates are higher in the range of $10^{-7}$ to $10^{-8}$ mm$^3$/N m. Wear rates in the $10^{-7}$ to $10^{-8}$ mm$^3$/N m range are considered low wear regime materials, often exhibited by solid lubricant coatings, such as diamond-like carbon and nano composite-alloyed MoS$_2$.\[21\] Therefore, the NC-textured ZnO grain nanolaminate film exhibits a very good wear behavior at both room and elevated temperatures.

A HRSEM image of annealed nanolaminate surface prior to sliding shown in Figure 1(b) reveals surface grain sizes of $\sim 30$ nm, in agreement with our prior XRD results.\[11,17\] The surface morphology of these nanoscopic grains is relatively smooth with atomic force microscopy determining the average root mean square roughness to be $3.45 \pm 0.07$ nm. Therefore, surface roughness effects would likely have an insignificant contribution to sliding friction and wear under larger real contact areas. After sliding at 0.72 GPa contact pressure, the deformed ZnO surface in Figure 1(c) exhibits ductile layering/smearing but not brittle cracking. This implies that the individual ZnO nanocolumns plastically shear. The deformed surface morphology indicates an additive shear across neighboring grains accumulating to the microscale. Figure 1(d) is a cross-sectional TEM image acquired along the FIB lift-out region shown in Figure 1(c). It shows a diffracting, plastically deformed 20–25 nm wide ZnO nanocolumnar grain with BSFs parallel to the sliding direction. It should be noted that a
careful FIB lift-out procedure was followed to circumvent Ga ion-beam damage during milling that could induce defect formation in the film. Therefore, the first step was to deposit Pt by using the electron-beam and then the ion-beam, which protects the TEM sample against beam damage. The second step includes milling and final polishing of the lifted-out sample using the Ga ion-beam at a conservatively low voltage of 5 keV and current at 70 pA to prevent Ga ion implantation.

Our DFT calculations of intrinsic basal and prismatic SF energies in wurtzite ZnO used the Vienna Ab Initio Simulation Package employing the projected augmented plane wave method.[23–25] Electron exchange and correlation are described within the generalized gradient approximation using the Perdew–Burke–Ernzerhof parameterization.[26] For a single unit cell (1 × 1 × 12 with dimensions of 3.29 × 2.85 × 63.66 Å), the energy cut-off was 532 eV and the k-point spacing used was <0.185/Å. Basal and prismatic SFs were introduced into SC ZnO crystal via a suitable displacement of two halves of the crystal. The faulted structures are relaxed until the forces on the atoms were less than 0.02 eV/Å. The stacking fault excess energy, also called the stacking fault energy (SFE), is calculated by subtracting total energies of the perfect ZnO crystal from the energy of the relaxed faulted system, and dividing this excess energy by the area of the stacking fault.

We now explain the microstructural defect evolution during film growth and after sliding. A missing or extra ZnO (0002) plane in growth BSFs may originate from incoherent boundaries between adjacent nanocolumns and/or condensation of vacancies or interstitials in NC (0002)-texture ZnO since the annealed ZnO layer is oxygen deficient. This could likely weaken the Zn–O bond strength and influence the energetics of dislocation nucleation and glide. The TEM image in Figure 1(d), and also weak beam dark field cross-sectional TEM, shows BSFs originating at low angle (≈15°) tilt grain boundaries. A cross-sectional HRTEM image acquired from the annealed, unworn ZnO layer shown in Figure 2(a) reveals a growth, intrinsic type I single BSF bordered by a PD. Type I intrinsic BSFs have only one violation in the stacking sequence.[16] Our DFT calculations show \( \cdots \cdots \cdots AaBbAaBbCcBbCc \cdots \cdots \) stacking sequence for type I BSFs as shown in Figure 2(b), where the capital and smaller letters denote a (0002) double layer occupied by Zn or O ions, respectively. The zinc blende structure forms locally with \( AaBbCc \) arrangement. This low-energy type I BSF is bordered by sessile Frank PDs with rigid body displacement (Burgers) vector equal to \( \frac{1}{6}[0223] \), shown in Figure 2(c). The intrinsic basal SFE was calculated to be 24 J/m², which is much lower and favorable than the calculated \{1010\}-prismatic SFE of 427 mJ/m². The average PD density bordering the BSF was based on counting the PDs in 10 different micrographs like the one in Figure 2(a). It is 1.5 ± 1 × 10¹¹/cm² for the as-deposited ZnO layer and 6.5 ± 1 × 10¹¹/cm² for annealed layers. Thus, annealing increases growth BSF likely due to an increase in oxygen vacancies determined by XPS, and correlates reduced friction to the increase in BSFs and PDs. In contrast, the higher friction observed for SC ZnO and NC-randomly orientated ZnO emphasizes the important role of grain boundaries as sources of BSFs and PDs in accommodating interfacial shear. The orientation of the PDs with respect to the sliding direction also has an effect as discussed below.

To determine if these mechanisms operate after frictional contact, cross-sectional HRTEM studies were done inside the ZnO subsurfaces of annealed nanolaminate with different NC grain orientations. Figure 3(a) shows
Figure 3. View of \{0002\} basal planes in a nanocolumnar ZnO grain. (a) Cross-sectional HRTEM image using \( g = (011\overline{1}) \) shows subsurface plastic deformation after frictional contact. SD is the sliding direction. (b) Corresponding FFT diffraction pattern shows that the basal planes are observed to be streaked along the [2\overline{1}1\overline{0}] beam direction, which is consistent with the presence of stacking faults running normal to the [2\overline{1}1\overline{0}] direction. (c) The identification of these dislocations is confirmed in the corresponding Fourier-filtered image using the \{0002\} diffraction spots, which demonstrate that each PD (shown by arrows) corresponds to one additional \{0002\} plane. The inset image in Figure 3(c) shows a higher magnification view of the PD denoted with the red arrow that terminates a BSF. The PD density increases by an order of magnitude to \(1.2 \pm 1 \times 10^{12}/\text{cm}^2\) as a result of frictional contact due to their nucleation at the nanocolumnar boundaries, which in turn increases the available pathways for dislocation glide. This averaged PD density was calculated by counting the number of PD from 12 similar TEM micrographs, like the one shown in Figure 3(c). The higher densities of growth BSFs also confine the slip to within each NC grain as inferred from non-observable gross-slip across multiple nanocolumnar grain boundaries and the absence of slip transmission across grain boundaries. Therefore, low friction and wear may be attributed to localized NC plasticity during sliding via a novel intrafilm shear velocity accommodation mode. This localized NC plasticity is single-crystal additive and accumulates to the microscale since the deformed surfaces, like the one shown in Figure 1(c), exhibit ductile layering/smearing.

Figure 4 shows another NC ZnO grain, but with \{011\overline{0}\} prismatic orientation. In contrast to the basal planes, the cross-sectional HRTEM image in Figure 4(a) shows no subsurface plastic deformation in the nanocolumnar grain after frictional contact. The corresponding FFT diffraction pattern shows that the prismatic planes are not streaked along the same [2\overline{1}1\overline{0}] beam direction, which is consistent with no stacking faults running normal to the [2\overline{1}1\overline{0}] direction. The absence of dislocations is confirmed in the corresponding Fourier-filtered image using the \{011\overline{0}\} diffraction spots, which means there are no prismatic stacking faults in the worn subsurface. This is consistent with our DFT calculated high SFE of \(\sim 427 \text{mJ/m}^2\) for the ZnO prismatic planes compared to \(\sim 24 \text{mJ/m}^2\) for the \{0002\}-basal SFE. Furthermore, these results imply that only basal slip is energetically favored, and that non-interacting slip systems translate to low interfacial shear and friction. A similar mechanism was postulated in HCP cadmium when the (0001) glide plane is parallel to surface and glide of the...
subsurface edge dislocations produce low shear.\cite{27} In a low SFE system like cadmium, dissociation of PDs into widely spaced partials reduces the critical resolved shear stress required for their glide on the fault plane. However, in the case of SC ZnO, cross-sectional HRTEM revealed cleavage cracks along (0002) planes, cause brittle fracture and larger wear particle generation leading to a higher friction.\cite{18} Since there are no low angle columnar grain boundaries for nucleation of BSFs and PDs, like in NC ZnO, we cannot achieve low interfacial shear. Higher friction and wear also occur in NC-randomly orientated ZnO grains, where many interacting slip systems would operate. Frictional contact in these randomly orientated grains likely caused the interaction and interlocking of slip systems, and ultimately localized hardening and brittle failure. This behavior is unlike other randomly oriented NC ceramics where grain boundary sliding and grain rotations contributed to enhanced plasticity.

It can be argued that the interfacial shear strength ($\tau_o$) obtained from Equations (1) and (2) during sliding is that between the Si$_3$N$_4$ counterface and ZnO layer. Because there was no detectable ZnO third body transferred to the Si$_3$N$_4$ counterface, we can assert that $\tau_o$ is not the value for Si$_3$N$_4$ counterface and ZnO layer. Our TEM analysis also supports this assertion by revealing the subsurface intrafilm shear along the ZnO {0002}-basal planes parallel to the sliding direction. Therefore, while there is relative sliding between the Si$_3$N$_4$ counterface and ZnO layer, it is the defective ZnO–ZnO basal plane interface that determines the friction coefficients and interfacial shear strengths. Thus, it is likely this intrafilm VAM is independent of the counterface material as long as it is not plastically deforming and forming a third body transfer film.

In summary, we have shown that it is feasible to achieve low friction and wear ceramic oxides by controlling the nanometer-scale structure. NC ZnO with low SFE {0002}-textured grains plastically deform via shearing of subsurface BSFs parallel to the sliding direction. The resultant novel intrafilm shear VAM yields exceptionally low interfacial shear strengths and friction and prevents brittle fracture commonly observed in conventional ZnO, and has broad implications to other defective NC ceramics. The comparisons with SC ZnO of identical texture and randomly oriented NC ZnO further support this VAM. Therefore, we have uncovered an unexpected trend wherein controlling the texture, grain size, and defect structure can potentially transform a conventional brittle oxide into a ductile one during sliding.

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