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Grain Boundary Sliding and Low Friction in BCC Metals

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We show evidence of low friction in BCC metals through molecular dynamics simulations and ultra-high vacuum experiments. This is shown to be correlated with grain boundary sliding (GBS) as the primary mechanism of deformation. Specifically, when grain sizes at the sliding interface are smaller than a critical, material-dependent value (on the order of 10-30 nm), a crossover occurs from dislocation mediated plasticity and Hall-Petch strengthening to GBS and interfacial softening. Results from simulations and experiments are quantitatively compared to a new predictive model of shear strength.

Keywords: tribology, BCC metals, grain boundary sliding, Hall-Petch, deformation mechanisms

Pure metal contacts typically show high friction and wear. This is especially true in the absence of oxidation, as oxide films can inhibit contact between the pure metals and lower adhesion. However, low friction in pure metals can be achieved (see Fig. 1) when shear-induced deformation results in a highly refined grain structure at the surface, with grains smaller than ~10 nm. The refinement is usually confined to a surface layer approximately 100 nm thick that acts as a sliding interface with reduced shear strength (see Fig. 2) [1,2].

While the phenomenon linking ultra-nanocrystalline grains to low friction has been discussed in the context of FCC metals, there have been few studies investigating similar behavior in BCC metals. The dislocation activity in BCC metals is distinctly different from FCC metals, and this often leads to brittle behavior in the former, as well as strong dependencies of their mechanical properties on strain rate and temperature. While these differences could lead to dramatically different friction mechanisms in BCC metals, we will show evidence that the grain-size dependent shear strength in both classes of metals is similar, particularly in the ultra-nanocrystalline (UNC) regime, where deformation is largely accommodated by grain boundaries via GBS.

We will discuss the evidence linking low friction and UNC grains in the context of a general map of friction regimes for metals that shows their tribological response as a function of time, temperature and stress [1]. This is followed by results from large-scale molecular dynamics simulations and ultra-high vacuum experiments that show this relationship in polycrystalline BCC Ta [3]. The results are placed in the context of a new, predictive model of shear strength in metals that describes GBS as dynamic amorphization of crystalline material [2]. This model successfully predicts the shear strength of BCC metals, as well as FCC metals and alloys, indicating that GBS is a universal mechanism in UNC metals.

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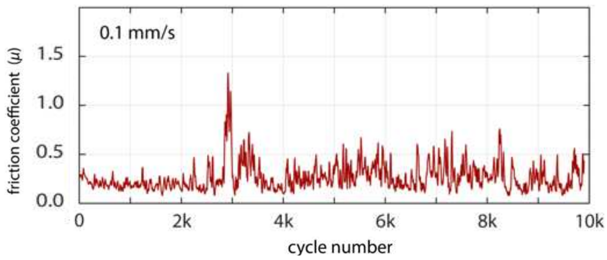

Figure 1: Friction coefficient of pure Ta contacts in ultra-high vacuum demonstrating low friction.

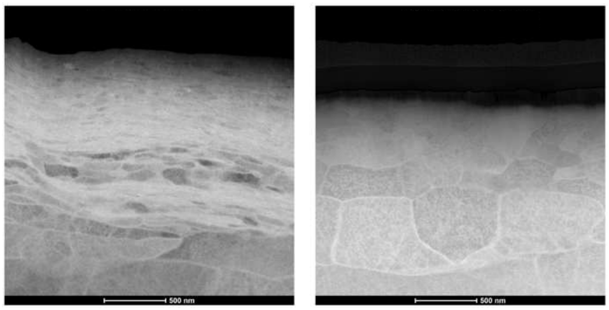

Figure 2: Cross-sectional transmission electron microscope images of polycrystalline Ta after sliding friction experiments. The low friction track is characterized by highly refined grains at the sliding interface (left image), while the high friction track is coarse-grained (right image)

References

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