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The Connection Between Microstructural Evolution and Metal Friction: Combining Experiments, Simulations and Theory into a Predictive Model

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The extraordinary mechanical properties of nanocrystalline metals are well-documented, though this class of materials often remains impractical for engineering design. This is due to instability in the grain size that manifests with the addition of even modest amounts of stress or heat. Sudden and unpredictable changes in grain size can dramatically reduce the strength of nanocrystalline metals and adversely impact tribological properties, i.e. induce high friction and multiple order-of-magnitude increases in wear rate. While it has been possible to achieve low friction and "ultra-low" wear with nanocrystalline metals – in one exceptional case that will be discussed, an alloy having friction coefficients and wear rates comparable to Teflon and diamond-like carbon, respectively – the ability to quantify and predict stability bounds has remained elusive until now, leaving engineers with only phenomenological models as design tools.

Based on complementary multi-scale experiments and molecular dynamics simulations, my work established fundamental correlations between microstructure evolution, deformation mechanisms and macro-scale friction. These correlations enabled the development of a new physics-based model able to predict the tribological stability thresholds of nanocrystalline metal contacts, exclusively as a function of materials properties, applied stress, and temperature. Based on these findings, it is possible to explain a long-standing causal misconception that higher hardness leads to higher wear resistance, explain the origin and regimes of validity of this notion, and provide a more reliable and quantitative mechanistic model for engineering design. We conclude with a look at tantalizing prospects for these ideas in the design of next-generation wind turbines, aerospace systems, and nanostructured materials.

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