Understanding the Mechanisms of Friction in Pure Metals, Alloys and Composites

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1. Introduction

Materials that perform well in electrical contacts usually exhibit high adhesion during frictional contacts. An excellent example of this phenomenon is pure gold, which has extremely low electrical contact resistance, but generally has a high friction coefficient. When composites are formed by alloying nanocrystalline gold with, for example, Ni or Co, the friction can be reduced while maintaining the low contact resistance. The mechanism for this is often attributed to increased hardness of the metal, but remains poorly understood. We will present the results of large-scale molecular dynamics (MD) simulations that study the tribological response of metallic films under a variety of sliding conditions. Results from pure metals, alloys, and composites will be used to elucidate the mechanism of friction in all three systems, with a particular emphasis on the causes of the reduction of friction in the alloys and composites.

2. Summary

The friction in pure metallic contacts is often high, with friction coefficients for macroscopic, low load contacts ranging from 0.5-2.0. In nanoscale contacts, the coefficient of friction is generally lower, with coefficients near 0.2-0.3. The addition of substituent atoms often lowers the friction coefficients substantially in both macroscale and nanoscale experiments. While the friction in pure metals is due to high adhesion, the reduction in alloys and composites is less well understood. The most common explanation is based on the increased hardness of the metal, but this has not been demonstrated conclusively to be the origin of the friction reduction. We demonstrate that the tribological mechanisms at work in metallic junctions is not related to the hardness of the metal, and can be ascribed to the sliding mechanisms that are active in each specific case.

In the case of pure metals, cold welding occurs at the junction. This is followed by stress-induced grain growth, which leads to the formation of a single grain across the interface. Sliding is then accommodated through dislocation controlled plasticity. In this situation, sliding occurs along the fcc slip planes (in the case of Au or Ag), which implies a commensurate contact, and therefore a higher coefficient of friction.

In composites or alloys (specifically those in which the substituent atoms have a different lattice constant compared to the host metal), the mechanism is different. In this case, while cold welding still occurs at the contact point, grain growth across the junction is suppressed, and sliding occurs along grain boundaries, resulting in a lower friction coefficient.

We demonstrate the two frictional mechanisms through a series of targeted, large-scale molecular dynamics simulations using validated models for the metals. In particular we show the grain growth in the pure metals, and the suppression in the alloys and composites. We then demonstrate that by designing a simulation in which the pure metals are forced to accommodate shear along grain boundaries, the friction coefficient is reduced to the same level as found in the alloys and composites.We also demonstrate that when the alloying is with a metal with a very similar lattice constant (i.e. Au and Ag), the grain growth mechanism is no longer suppressed, and friction returns to a level similar to that found in the pure material.

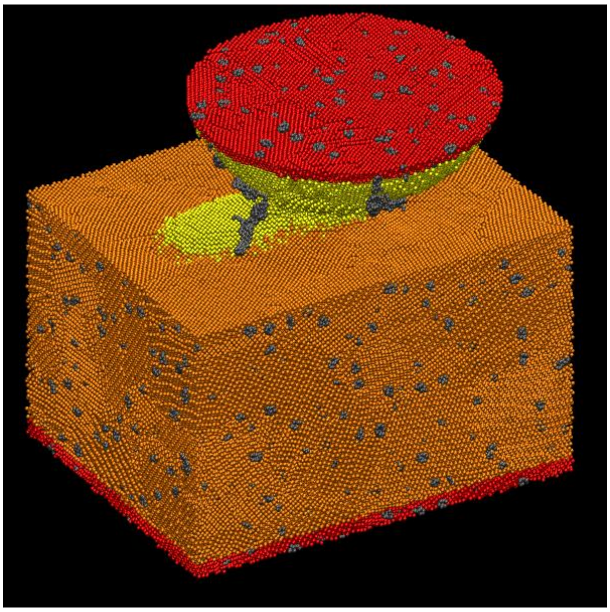

Figure 1 Snapshot of simulation in which a 10nm tip of AuC composite slides on an AuC composite substrate. Gold atoms are shown in red, orange and yellow, while carbon atoms are shown in gray.

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