Mechanical Wear Behavior of a Model Metallic Glass Asperity via Molecular Dynamics

by

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ABSTRACT

The macroscopic wear rate has been described quantitatively by the Archard's Wear Law. Here, we investigate the validity of Archard's Wear Law at the nanoscale level. This study is performed using molecular dynamics with simulated AFM tips sliding on a single asperity substrate under different loading conditions and tip geometries. We examine the wear of the amorphous AFM tips under both constant pressure and constant force loading conditions. Unlike Archard's wear law which is independent of the contact area, it was found that the rate of tip wear is contact area dependent. We have identified a critical stress separating a low wear rate regime (atomic wear regime) and a high wear rate regime (plastic-flow wear regime).

To further understand the plastic flow regime, an extensive analysis into the yielding behavior of a bulk amorphous glass is performed. The yielding of metallic glasses (MGs) is generally considered to be dependent on pressure or normal stress, which is usually described by the Mohr-Coulomb yield criterion. Experimentally, the orientation of the shear band angle or fracture angles in MG is roughly 40^o to 42^o in uniaxial compression and 50^o to 59^o in uniaxial tension, both with respect to the loading direction. However, the amounts of deviation from the maximum shear stress direction (45^o) under uniaxial tension and compression are quite different, which seem to be inconsistent with the Mohr-Coulomb yield criterion. Here we carried out simulations to study the incipient plasticity of model Dzugutov glasses subjected to various uniaxial and biaxial stress states. The yield points are defined as the sharp rise of atoms participating in non-affine deformations. The yield surfaces thus created agree well with the Mohr-Coulomb yield criterion. Furthermore, the orientations of the embryonic shear bands (instead of the fully-grown shear bands, or fracture planes) are measured, which also follow predictions based on the Mohr-Coulomb criterion. Using the angles of the embryonic shear bands, we are able to extract a value for the normal stress coefficient which is used in our model for predicting the slipline angle during plastic wear. We then compare the theoretical predictions to our measured values, and discuss key observations and trends which are useful for predicting and describing the wear of amorphous solids.