Molecular Dynamics Simulations of Dynamic Friction and Mixing at Rapidly Moving Material Interfaces

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Friction studies are important in applications to high-speed machining and ballistic penetration modelling, two areas where it is important to understand the behaviour of rapidly moving interfaces. Gaining insight into the velocity dependence of the effective tangential force, and its time-evolution, under various external loads is also of particular interest. Previous studies [1, 2, 3], have shown that for metals, a substantial velocity weakening occurs, i.e., a decrease in the friction stress with velocity, and this has been attributed to melting. Furthermore, experimental studies [4] have shown the development of characteristic micro structural changes during ductile metal sliding, which is distinguished by a very highly strained plastic region near the interface and a nano-crystalline region at the interface. The details of the phenomena that occur along and across the interface between two materials cannot be modelled by continuum mechanics, but instead a microscopic analysis of these phenomena is required.

The present study concerns molecular dynamics (MD) simulations of dynamic friction at Cu/Ag interface. MD simulations using the Embedded Atom Method (EAM) interatomic potentials have been performed for a box containing $1.3 \cdot 10^6$ atoms. Compression forces of the order of 5.1GPa have been applied to Cu(010) and Ag(010) as well as sliding friction velocities of up to 1Km/sec in the $\langle 100 \rangle$ crystallographic direction.

The aim of this work is to confirm the connection between velocity weakening and structural transformation of nano-crystalline materials. The frictional force versus relative sliding velocity for the two interfaces reveals a linear region at low velocities and a highly localised plastic deformation region at high velocities with the frictional force decreasing with velocity. The study also tries to shed light on the temperature dissipation in the proximity of the interface and its relationship with atomic diffusion. The temperature distribution across the interface of the two materials exceeded the melting point, especially at velocities greater than 500m/s. Mixing of the two materials was also observed at the sliding interface with the mixing layer width increasing when increasing the sliding speed.

References

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