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The Evolution of Tribomaterial During Sliding: A Brief Introduction

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Abstract This brief introductory article summarizes key findings from experiments and from computer simulations concerning the dramatic changes that commonly occur adjacent to sliding interfaces. We conclude that a wide range of observed features depends on a few basic processes (plastic deformation, interactions with the environment (including the counterface) and mechanical mixing) and that sliding leads to flow patterns similar to those expected in fluid flow.

Keywords Sliding · Tribomaterial · Vorticity · Mechanical mixing

It is now widely recognized that sliding dramatically changes the material adjacent to the sliding interface. The modified material, simply called 'tribomaterial' here, has been given many other names, including the following: amorphous layer, Beilby layer, transfer layer, fragmented layer, highly deformed layer, glaze layer, white-etching layer, nanocrystal layer, third body [1] and mechanically mixed material. Sliding commonly produces tribomaterial that is both structurally and chemically different from the bulk material [2, 3]. The development of this tribomaterial influences both friction and wear and suggests that simple models, e.g., familiar adhesion, delamination, fatigue and

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S. Karthikeyan Materials Engineering, Indian Institute of Science, Bangalore 560012, India e-mail: karthik@materials.iisc.ernet.in oxidation models, are not adequate for understanding and controlling sliding behavior.

Experimental observations during and after sliding, combined with computer simulations [2–16], show why our understanding of sliding processes has been elusive. In contrast to abrasion, which can be described in terms of geometry, relative hardness, indentation and microcutting [17], sliding commonly involves all of the following: large plastic strains and strain gradients, high strain rates and strain rate gradients, mechanical mixing of components



Fig. 1 Schematic of a simple system consisting of a harder material A sliding on a softer material B. Gradients of strain and strain rate evolve together with local structural features as sliding and plastic deformation proceed. Nearest to the sliding interface, a uniform or patchy layer of tribomaterial develops. It can be nanocrystalline or even amorphous, and its composition may be different from that of either bulk material. Typically, the boundary between the tribomaterial and the adjacent highly deformed material is sharp, suggesting that more than simple thermal diffusion is involved in its formation [1]. Wear debris particles commonly have the same structure and composition as the layer of tribomaterial [2]

Mechanically-mixed matl. (Bulk metallic glasses)



SEM image of longitudinal cross-section of $Zr_{41,2}Ti_{13,8}Cu_{12,5}Ni_{10}Be_{22,5}$, tested in air

Fig. 2 Back-scattered electron (BSE) image of a longitudinal crosssection of a wear track formed during self-mated sliding of a bulk metallic glass (BMG) in air (vertical pin/disc, 1.1 kgf, sliding speed 0.05 m/s [7]). The BSE image provides atomic number contrast, and the uniformly darker tribomaterial is found to contain oxygen. Plastic deformation of the adjacent BMG causes a decrease in hardness compared with the original material. When sliding is done in vacuum, such softening is the dominant effect, and the layer with oxygen mixed in is absent. In air, the harder oxygen-containing material is brittle, and that tribomaterial is the source of wear debris particles having the same structure and composition

Evolution of microstructure: Marker displacement

Two experimental examples (crystalline)



Fig. 3 Two examples of longitudinal cross-sections of wear scars after sliding against a hard steel. The oxygen-free high-conductivity (OFHC) single-phase copper specimen shows a pattern of dislocation cells that become smaller as plastic strain increases in this workhardening system. The grain boundary serves as a displacement marker. At the surface is a nanocrystalline layer containing a small amount of iron from the counterface. The two-phase Pb–Sn specimen was directionally solidified to produce lamellae that served as displacement markers. Again, the plastic deformation is largest near the surface, where the material work-softens and the structure coarsens with time

Fig. 4 The upper three figures show development of vorticity that is expected from consideration of Kelvin-Helmholtz instability [21, 22]. The lower three figures show a sequence of snapshots from a simple molecular dynamics (MD) simulation in 2-D of selfmated sliding of a twocomponent amorphous material modeled with Lennard-Jones (L-J) potentials. The comparison, together with observation of the full sequence in movie format, suggests that instabilities during sliding lead to vorticity that is responsible for mechanical mixing. Such a process is much faster than one that relies on normal diffusion [3, 6–16, 18]

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Fig. 5 A single frame from a simple 2-D MD simulation [15] using L–J potentials to model the sliding of two close-packed crystalline materials. The parameters are chosen so that A and B are similar but A is slightly harder than B. Vorticity is depicted by *shading (color in on-line version)* and by the *small arrows*, each of which is proportional to the velocity of one atom. Mixing occurs in the zone with highest vorticity. The image corresponds to conditions that approach steady state. A very similar pattern develops at long times when A slides against A, but for that case there is initially much surface roughening and deformation far from the interface before the system settles down and becomes like that shown in the figure above

A wide range of observed features depends on a few basic processes: plastic deformation, interactions with the environment (including the counterface) and mechanical mixing. These processes are not adequately incorporated in traditional models [19, 20] of friction and wear. The composition and properties of the mixed material can vary widely for different materials and sliding conditions, so there can be a broad range of sliding behavior despite the involvement of the same basic processes. Special cases, e.g., effects of phase transformations, particle cracking, degradation of lubricants, etc., contribute to sliding behavior, but within the same broad framework.

Molecular dynamics (MD) simulations suggest for both crystalline and amorphous materials that sliding leads to flow patterns similar to those expected in fluid flow [6–16]. Mixing occurs when a Kelvin–Helmholtz shear instability [21, 22] leads to vorticity, and the size scale of the vortices is similar to that of grain sizes in nanocrystals. This



[2].

Fig. 6 a Schematic of 3-D MD simulation using EAM potentials for sliding of FCC Cu against BCC Fe [16]. Periodic boundary conditions are used in the *x* and *z* directions. Reservoir regions are maintained at low temperature, so they serve as heat sinks for frictional heat. These were also used for the earlier 2-D simulations using L–J potentials.

The average velocity of atoms in the reservoir regions is held constant. **b** Initial configuration of Cu and Fe atoms for a particular orientation of each crystal relative to the x, y, z coordinates. Markers for displacement measurements are easily included by coloring selected atoms



V =500 m/s, t = 32.9 ps, slid 16 nm

V =400 m/s, t = 30.25 ps, slid 12.1 nm

Fig. 7 a Configuration of Cu and Fe atoms after sliding, with initial orientations as shown in Fig. 6b. Plastic deformation occurs only in the Cu. The sliding interface shifts into the Cu, indicating transfer of Cu to the Fe. Part of the transfer material is an epitaxial layer of BCC Cu on Fe [16]. Vorticity has dispersed the marker atoms in the vicinity of the sliding interface. **b** Configuration of Cu and Fe atoms

after sliding. The orientation of the Fe crystal is the same as in Figs. 6b, 7a, but the initial orientation of the Cu crystal is chosen so that dislocation motion is not favored. As a consequence, material near the sliding interface amorphizes and some Fe atoms mix into the Cu. The amount of transfer material is greater than in Fig. 7a, but the portion that is epitaxial BCC Cu on Fe is less [16]

Fig. 8 a Initial configuration for a bicrystal of Cu sliding against an Fe crystal (same orientation as in Figs. 6b, 7b). b Nanocrystalline structure produced after sliding for the initial configuration shown in Fig. 8a. The bicrystal arrangement allows more extensive deformation in the Cu than for cases involving single crystals of Cu, even at low sliding velocities. The sequence of events includes propagation of shear bands, formation of epitaxial Cu and dynamic recrystallization [16]



V = 300 m/s, t = 0 ps, slid 0 nm

V =300 m/s, t = 88 ps, slid 26.4 nm

correlation suggests that vorticity drives mechanical mixing and is at least partially responsible for the development of nanocrystalline material during sliding and during other processes involving severe plastic deformation. Recent results suggest that the formation of nanocrystals may be influenced by vorticity-driven dynamic recrystallization [16]. The disappearance of markers is also associated with vorticity. The simulations show dramatic rearrangements of structure when the normal load is removed or when sliding ceases [14, 16]. These observations raise important questions about conclusions based on even the most careful post-test observations of tribomaterial.

In all cases reported, the tribomaterial that develops during sliding is clearly different from the bulk material in the contacting materials. Therefore, a focus on the tribomaterial and its properties will be needed to develop friction and wear models that are physically reasonable and ultimately useful. In the case of wear models, the fracture characteristics of the tribomaterial need to be incorporated.

Figures 1, 2, 3, 4, 5, 6, 7 and 8 provide experimental and simulation examples of structures produced during the sliding of materials. The tribomaterial examples given here are in the regimes of nano- and micro-structure. However, similarities with structures produced in bubble rafts [23] and in structures observed after slip associated with earthquakes [24] suggest that the processes described here are quite general and may be important over a wide range of size scales, from the nanoscale to the macroscopic.

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