Frictional interactions at high velocity ductile metal interfaces

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Abstract. We have examined the effect of evolution of grain morphology on the frictional force at polycrystalline Al-Al and Al-Ta interfaces as a function of grain size and sliding velocity. We present the results of 8M, 26M and 138M particle NonEquilibrium Molecular Dynamics (NEMD) simulations for grain sizes of 13 and 20 nm. Sample sizes consisted of $3 \times 3 \times 3$ and $5 \times 5 \times 5$ grains on each side of a sliding interface. We have considered sliding velocities from 20 to 4000 m/s. For velocities below a size dependent critical velocity above which a fluid layer forms, we find enhanced grain coarsening leading to a highly strained, graded final steady state microstructure that exhibits a dynamic morphology for times greater than 5-10 ns. We find that the frictional force is insensitive to the initial grain size distribution due to the evolution of the initial distribution to a new nonequilibrium steady state. We discuss the relationship of these results to single crystal interfaces and the mechanisms for grain size and shape evolution.

1. Introduction
The frictional force between two ductile metals as a function of sliding velocity depends on a number of parameters, including local temperature, pressure, dislocation densities, and defect and impurity concentrations. Another material parameter is the grain size distribution. In many cases for ductile metal sliding, the local grain structure is transformed during sliding to one that is significantly different from the original grain morphology, exhibiting sub-grain transformation to microstructures characterized by very large plastic deformation and elongation in regions of order tens of microns from the sliding interface [1]. This micro/nano structural transformation may also be coupled to material mixing [2]. The fact that the local interfacial microstructure in the dynamic steady state differs from the bulk material microstructure presents a challenge to constructing a realistic model for the frictional force under dynamic loading conditions characterized by large strains and strain rates. To examine the consequences of initial grain size distribution on the velocity dependence of the frictional force we have considered two interfacial systems, Al-Al and Al-Ta, and performed large scale NonEquilibrium Molecular Dynamics (NEMD) simulations for a range of velocities. In the following sections we describe the details of the simulations for systems with 13 nm and 20 nm initial average grain sizes at nominal pressures of 15 GPa. Section 2 describes the simulation method and boundary conditions. Section 3 describes the evolution of microstructure and the velocity dependence of the frictional force. Section 4 discusses these results in the context of single crystal simulations.
2. Simulation method

The NEMD method we employ to determine the frictional force has been used previously to study the velocity dependence of the frictional force at single crystal interfaces [3]. We consider a computational volume with dimensions \((L/2, L, L/2)\) in the \((x,y,z)\) directions with periodic boundary conditions in \(x\) and \(z\). The initial sliding interface is at \(y = 0\) and sliding is along the \(x\)-direction. In a small reservoir region comprising typically \(10 - 20\) lattice planes in the \(y\)-direction we apply a time-dependent external force at each time step, uniformly to each atom in the reservoir region, \(F_i(t) = F_{0i}(t)\) such that \(\langle v_y\rangle_{Res} = \pm u_p\) in the reservoir regions at \(y = \pm L/2\). We also thermostat the temperature in the reservoir region so that \(\langle T\rangle_{Res} = T_0 = 300\) K. We equilibrate the sample for 50 ps at zero velocity and then apply an initial velocity distribution \(v_y(y > 0) = +u_p\) and \(v_y(y < 0) = -u_p\) to within thermal fluctuations at \(T = 300\) K. With these boundary conditions and initial conditions the classical equations of motion are integrated using the parallel SPaSM NEMD code developed by Lomdahl et al. [4]. Time steps are typically 3 fs. The system evolves under the influence of Embedded Atom Method (EAM) potentials used in previous work for single crystal sliding [5]. In the non-reservoir regions no external forces are applied and the atoms are not thermostatted. For long times, \(F_i(t)\) reaches a steady state average value \(F_i\) and the frictional force per unit area is \(f = N_{Res} F_i / A\) where \(N_{Res}\) is the number of reservoir atoms and \(A\) is the area, \(A = L^2/4\).

The polycrystalline samples have been constructed by a sequence of annealing at a volume corresponding to the density of Al (and Ta for the Al-Ta interface) at 300 K and 15 GPa. The initial polycrystal was constructed using a Voronoi procedure and the annealing procedure produced an approximately stress free sample at \(T = 300\) K and \(P = 15\) GPa. A similar procedure has been used in simulations of polycrystalline materials by Kadau et al. [6]. The samples for Al-Al sliding were formed by taking an annealed sample of size \((L/2, L/2, L/2)\) for the upper \((y > 0)\) material and rotating this sample by \(\pi/2\) about the \(y\)-axis for the lower \((y < 0)\) material.

3. Results

We present the results of polycrystalline simulations for Al-Al and Al-Ta interfaces. For the Al-Al 13 nm grain size sample, \(L/2 = 38.5\) nm, \(N_{\text{atom}} = 7.78 \times 10^6\), \(N_{Res} = 5.15 \times 10^5\) with 27 grains initially on either side of the interface. For the 20 nm grain size sample, \(L/2 = 100\) nm, \(N_{\text{atom}} = 1.38 \times 10^8\), \(N_{Res} = 2.13 \times 10^6\) with 125 grains on either side of the interface. This was also the approximate size for the Al-Ta 20 nm grain size simulations. We also considered a smaller 19.3 nm sample with \(L/2 = 57.75\) nm with 27 grains on either side of the interface and \(N_{\text{atom}} = 2.65 \times 10^7\), \(N_{Res} = 1.27 \times 10^6\). Figure 1 shows the initial configuration and the configurations at 3, 5, 7 and 10 ns for the Al-Al 20 nm grain size simulation with relative velocity \(v = 2u_p\) = 100 m/s and \(L/2 = 100\) nm. The colours correspond to the orientation of the grains in an OIM image. The behaviour of grain growth seen in these figures is generic for all simulations when the relative velocity is smaller than a critical velocity \(v_c\). The grains near the sliding interface grow and elongate due to the very large plastic deformation generated at the interface. At longer times we find that when shear strains reach magnitudes of order 2-3 near the interface, the grain structure refines to smaller grain sizes (but larger than the initial grain size) and that this behaviour repeats in a quasi-periodic manner. This is shown in figure 1e where the tangential force per unit area versus time is plotted. The oscillations correspond to growth followed by refinement. During the course of sliding the actual sliding interface, the point in \(y\) where \(\langle v_y(y)\rangle = 0\), meanders above and below \(y = 0\) due to this complicated grain dynamics and an approximately linear velocity profile develops in the \(y\) direction through a process region of order several tens of nm.
The average effect on the frictional force due to grain dynamics is shown in figures 2 and 3 and may be discussed in terms of two critical velocities introduced in the study of single crystal sliding [3]. There, a lower critical velocity, \( v_c \), and a higher critical velocity, \( v_{c1} \), were introduced with \( v_c \) defined by

\[
\nu_c = 4 \frac{\kappa(T_m, T_0)T_m}{f_L(T)} (1 - \frac{T_0}{T_m})
\]

where \( \kappa \) is the thermal conductivity and \( \kappa(T_1, T_2) \) is the average thermal conductivity between \( T_1 \) and \( T_2 \), and \( f_c \) is a critical force per unit area. For \( v > v_c \), \( f = f_c(v/v_c)^\theta \) and for \( v \geq v_{c1} \geq v_c \), a Couette fluid layer forms whose thickness increases with velocity with the interface temperature, \( T(0) \), increasing with \( v \) and independent of \( v_c \) [3]. For \( v \leq v_{c1} \leq v_c \), \( T(0) \) is almost constant and near the melting temperature \( T_m \). Figure 2 shows the frictional force per unit area as a function of \( v/v_c \) and figure 3 the homologous interface temperature, \( T(0)/T_m \) as a function of sliding velocity. The positions of the upturn in figure 3 occur at \( v_c \) that differs due to the different sample sizes corresponding to different values of \( L \).

**Figure 1.** OIM maps for Al-Al 20 nm grain size. \( v = 100 \, \text{m/s}, \, L/2 = 100 \, \text{nm} \). (a) \( t = 0 \), (b) \( t = 3 \, \text{ns} \), (c) \( t = 5 \, \text{ns} \), (d) \( t = 7 \, \text{ns} \) and (f) \( t = 10 \, \text{ns} \). The black dashed line indicates the initial position of the interface. The white dashed line indicates the position of the zero velocity point averaged over planes perpendicular to the normal direction. Tangential force per unit area vs. time is shown in (e).
We have also considered an Al-Ta interface with the same (20 nm) grain size and sample size as the Al-Al interface described above. Figure 4b shows a comparison of the time-dependence of the frictional force for $v = 100$ m/s and figures 4a and 4c show OIM images for the Al-Al and Al-Ta 20 nm polycrystalline interfaces at $t = 16$ ns.

4. Discussion
The simulations presented above have shown several interesting similarities and differences between the frictional behaviour of polycrystalline and single crystal compressed interfaces. The behaviour of both polycrystalline samples for $v > v_c$ is very similar to the single crystalline results. Figure 2 shows
that \( f \), the frictional force per unit area, depends upon velocity approximately as \( (v/v_c)^{-\beta} \). In this regime the interfacial temperature is near or above the melting temperature. Above a second critical velocity, \( v_{c1} \), the interfacial temperature divided by the melting temperature as a function of velocity is the same for both single and polycrystalline samples. For velocities above \( v_{c1} \) a three dimensional fluid Couette layer forms in all cases which is the underlying reason for this identical behaviour. For velocities below \( v_c \), the frictional behaviour of single crystal and polycrystal differs. The single crystal incommensurate interfaces have a frictional force which increases with velocity whereas the polycrystalline samples with a distribution of orientations and grain boundaries have a frictional force which decreases with velocity and has a low velocity value of order the material flow stress. In this lower velocity regime the grain growth determines the final average frictional force with similar values for both grain sizes. In the present simulations the grain growth is driven by the large plastic deformation that develops near the interface as is evident from detailed examination of figures 1 and 4. The magnitudes of plastic deformation may be estimated from the distorted regions near the interface and the local velocity profiles. They become of order 2 to 3 for the points in time at which grain refinement occurs in figure 1e.

It is often assumed for a heterogeneous material interface in dry sliding that the frictional properties are determined by the weaker of the two materials. The results in figure 4 are a confirmation of this presumption. The deformation occurs in the aluminium with similar grain growth behaviour to the Al-Al interface and the time dependence shown in figure 4b is essentially identical for both Al-Ta and Al-Al interfaces. The dynamics of grain evolution seen in these polycrystalline simulations provide important information for the development of larger length and time scale theories of the frictional force between compressed ductile metal interfaces and the general velocity dependence of the frictional force for ductile metal interfaces in dry sliding.

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