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Institutional Computing Annual Report – W11_Friction

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Abstract

The IC W11_Friction program has as a goal the fundamental understanding of the physical mechanisms which determine the macroscopic frictional force between ductile metals for arbitrary compressions and relative velocities. The high performance computing platforms have allowed detailed understanding of physical mechanisms: elasticity, anharmonicity of phonons, plastic deformation, phase transitions and melting, and grain structure including grain growth and refinement. The method used has been Non Equilibrium Molecular Dynamics (NEMD) using the SPaSM parallel code developed at LANL. The results of these simulations have resulted in a scaling model for the metal-metal frictional force.

Introduction

NEMD simulations, most recently on Roadrunner, Cielito and Cielo, have focused on metallic interfaces driven at relative velocity v at material pressure P . These conditions are enforced at the normal boundaries of the simulation cell that are located at distances $\pm L/2$ from the sliding interface between two metals. The normal load is imposed at this boundary to control P and a tangential force F_t per atom in a small reservoir region at the boundary that is time dependent and enforces a constant $\pm v$ velocity in the tangential direction. The temperature in the reservoir region is thermostatted to a temperature T_0 . Under these boundary conditions (with periodic boundary conditions in the sliding plane directions) a steady state is achieved in the long time limit that results in an average frictional force. In certain cases we have employed a fixed volume boundary condition as well. Figure 1 shows a characterization of the NEMD simulation cell. System sizes have evolved from 1 M atoms to currently approximately 150 M atoms and simulation times from 1 ns to approximately 30 ns for which dimensions are of the order $0.1 \mu\text{m}$ cubed on Cielo. Current simulation sizes (150 M atoms) have allowed consideration of near mesoscopic grain sizes consisting of 125 grains of size 20nm on either side of an Al-Al sliding interface.

Fig. 1 A typical simulation sample for an NEMD friction simulation. Reservoir regions are at the top and bottom of the system. $F_t(t)$ is the time-dependent tangential force applied such that the resulting average velocity in the reservoir regions is $u_p=1/2v$. A constant temperature is also applied to the reservoir regions.

Synopsis of Results

The results of the computational program are the basis for a model of the metal-metal frictional force that is characterized by two critical velocities, v_c and v_{c1} [cf. references] with $v_c < v_{c1}$, and a critical frictional force per unit area f_c :

$$v_c = \frac{4\bar{\kappa}T_m}{f_c L} \left(1 - \frac{T_0}{T_m}\right)$$

$$f = f_c \left(\frac{v}{v_c}\right)^{-\beta} \quad (v \geq v_c)$$

Here, T_m is the bulk melting temperature, $\bar{\kappa}$ is the average thermal conductivity between T_0 and T_m , $L/2$ is the reservoir-interface distance and β is approximately $3/4$. The upper critical velocity, v_{c1} , determines the onset of the formation of a Couette flow region at the interface for $v \geq v_{c1}$ with the interfacial temperature, T_{int} , greater than T_m . For $v < v_c$, the details of the frictional force depend upon micro(nano)-structure. The above expressions are for a homogeneous material interface. Similar expressions obtain for a heterogeneous interface. The two figures below show the results for single crystal Al-Al interfaces of various orientations as well as very recent polycrystalline simulations for grain sizes of 13nm and 20 nm. The dashed line in fig. 2 corresponds to $\beta = 3/4$.

Fig.2 Frictional force per unit area for Al-Al single crystal and polycrystalline interfaces showing velocity scaling for $v > v_c$.

Fig.3 Interfacial temperature for Al-Al single crystalline interfaces. The upper critical velocity is approximately 900 km/s.

The 20 nm polycrystalline simulations are the largest NEMD simulations ever done for polycrystalline materials beyond the inverse Hall-Petch size limit and have shown interesting new phenomena. First, the low velocity frictional force is markedly higher than that for the single crystal incommensurate interfaces for $v < v_c$. Secondly, there are dramatic differences in the steady state grain structure from the initial grain structure. Thirdly for $v < v_c$, the dynamic steady state achieved at long times is characterized by a quasi-periodic coarsening of elongated near interface grains followed by dynamic refinement when plastic strains reach magnitudes of 150 %, this coarsening and refinement oscillation persisting during the very long times of 30 ns in these simulations. An indication of this behavior is shown in Fig. 4. These polycrystalline simulations are being actively pursued both for the homogeneous and heterogeneous interfaces and are the basis for a larger length scale and longer time scale sub-grid hydro model.

Fig 4. The quasi-periodic dynamic growth and refinement of grains for a Al-Al 20 nm grain size sample sliding at $v= 100$ m/s and $P= 15$ GPa as a function of time compared to the frictional force per unit area vs. time.

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Frictional Interactions at Ductile Metal Interfaces: Large scale NEMD Simulations Supporting Model Development

The model correctly reproduces the very large scale SPaSM NEMD results for single and polycrystalline materials. An example for Al-Al interfaces at 15 GPa is shown below for the frictional force and the interfacial temperature.

Frictional Interactions at Ductile Metal Interfaces: Large scale NEMD Simulations Supporting Model Development

Recent polycrystalline Al-Al 20 nm grain size simulations (150M atoms for 30 ns) on Cielo have shown remarkable grain coarsening and refinement transitions in the steady sliding state driven by the very large plastic strains achieved at the sliding interface. The interfacial frictional force per unit area (GPa) vs time (ns) and the time dependent transitions are shown below.