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Friction and Shear Strength in Metals via Atomistic Simulations

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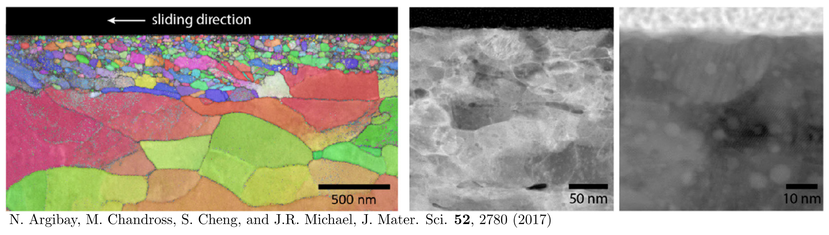
Introduction

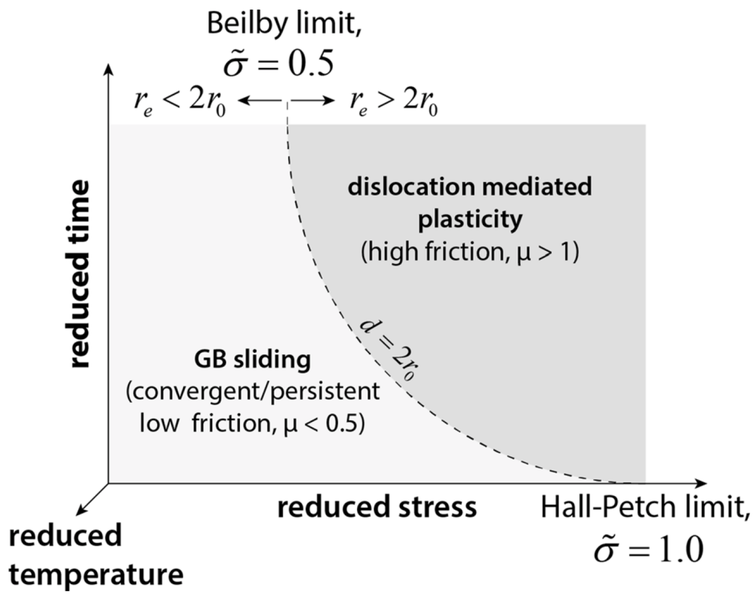
The friction between bare, metal-on-metal contacts is traditionally understood to be high, with friction coefficients near or exceeding $\mu = 1.0$, accompanied by significant galling and wear. Despite this, metals remain the only feasible materials for numerous essential engineering applications and component designs due to their favorable mechanical and structural properties. However, particular investigations of metal-on-metal friction have reported that it is possible to achieve remarkably low-friction behavior ($\mu < 0.5$) on bare surfaces. For pure, bare metals sliding in inert environments, it defies convention that the friction behavior should be anywhere below values commensurate with strong and rapid interfacial bonding. This unusual low-friction regime appears to be associated with the formation and persistence of a stable nanocrystalline surface film, with grain sizes well below 100 nm.



N. Argibay, M. Chandross, S. Cheng, and J.R. Michael, J. Mater. Sci. **52**, 2780 (2017)

A Friction Model

Recent progress in understanding and predicting this low-friction regime for Au, Ag, Cu, and other FCC metals during sliding contact has led to a model that links the microstructure (grain size) evolution and distinct plasticity mechanisms occurring at the interface to the resulting friction behavior.



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$$r_e = \frac{r_o}{1-\frac{\sigma}{\sigma_\infty}}$$

$$\sigma_\infty = \frac{2\gamma_{\mathrm{sf}}}{b}$$

$$r_o = \frac{Gb^2(2+\nu)}{8\pi\gamma_{\mathrm{sf}}(1-\nu)}$$

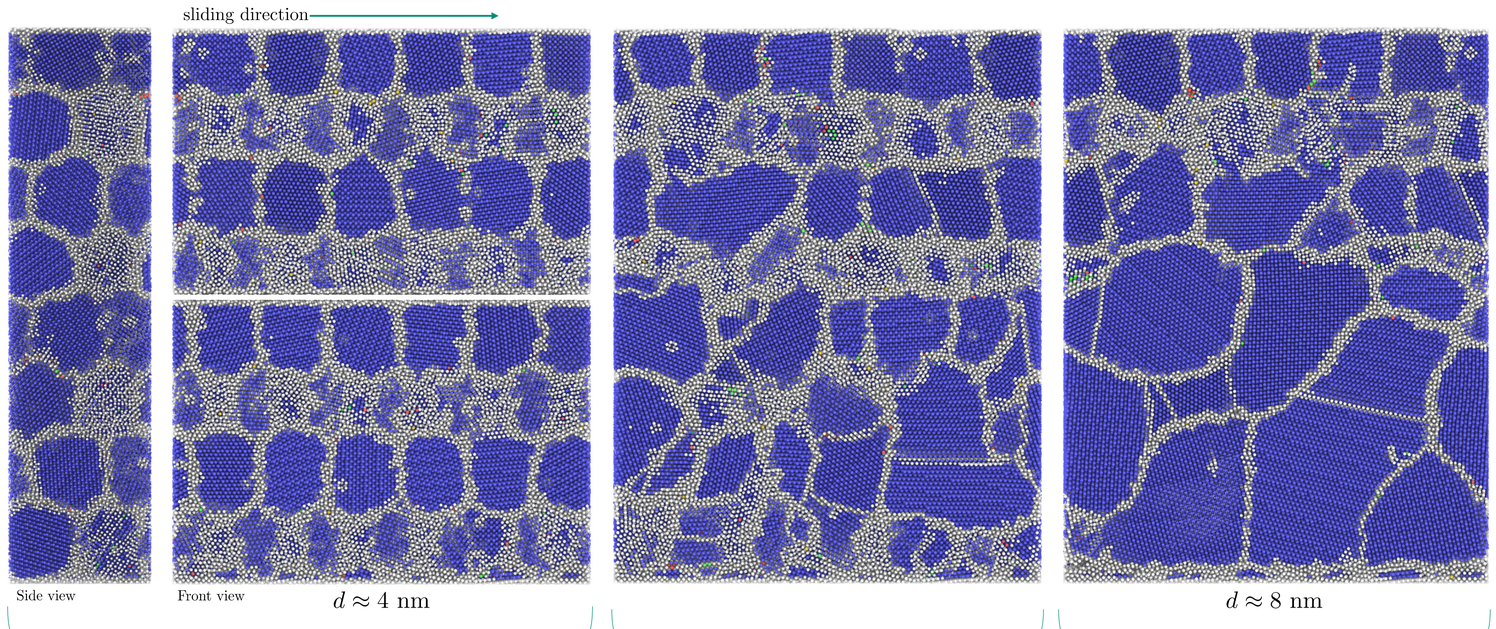
Definition	Variable
Resolved shear stress	σ
Hamilton stress (von Mises)	σ_h
Theoretical shear strength	σ_∞
Reduced stress σ/σ_∞	$\tilde{\sigma}$
Stacking-fault energy	γ_{sf}
Average grain boundary energy	γ_{gb}
Dislocation splitting distance	r_e
Equilibrium splitting distance	r_o
Burgers vector	b
Shear modulus	G
Poisson's ratio	ν
Mobility	M_o
Rate of grain growth	v_{gb}
Activation Energy	Q
Grain size	d
Activation volume	V
Hertzian contact radius	a
Normal Force	F_N

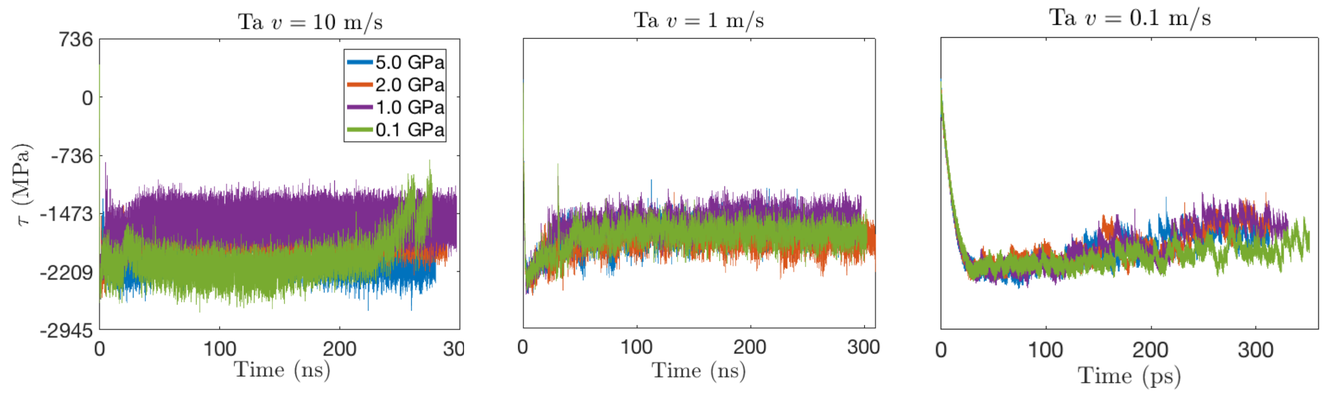
$$\sigma_h = \frac{3F_N}{2\pi a^2}\left(\frac{1-2\nu}{3} + \frac{4+\nu}{8}\pi\mu\right)$$

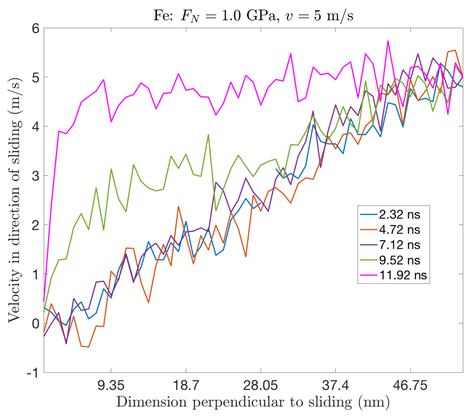
$$v_{gb} = \frac{\partial d}{\partial t} = \frac{2\gamma_{\mathrm{gb}}}{d} M_o \exp\left(\frac{-Q}{k_B T}\right) \exp\left(\frac{\left(\sigma_h - \frac{1}{2}\sigma_\infty\right) V}{k_B T}\right)$$

Here we present preliminary results to extend the FCC friction-regime map to BCC metals using molecular dynamics simulations of polycrystalline Ta and Fe slabs during sliding contact.

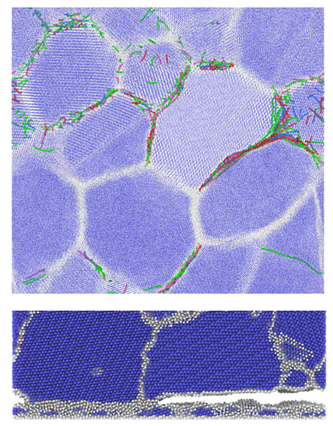
Nanocrystalline Tantalum and Iron

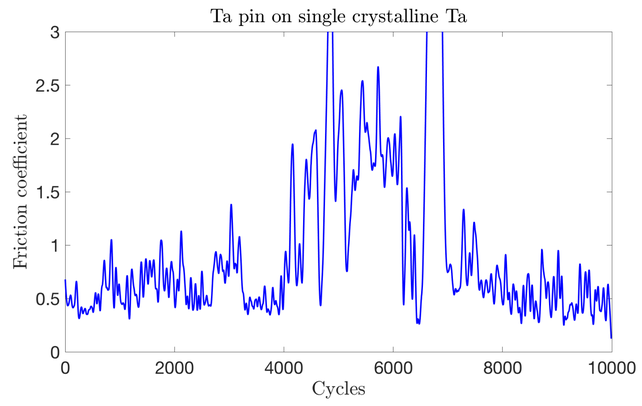




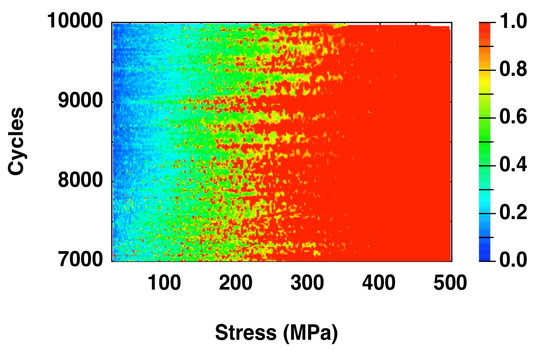


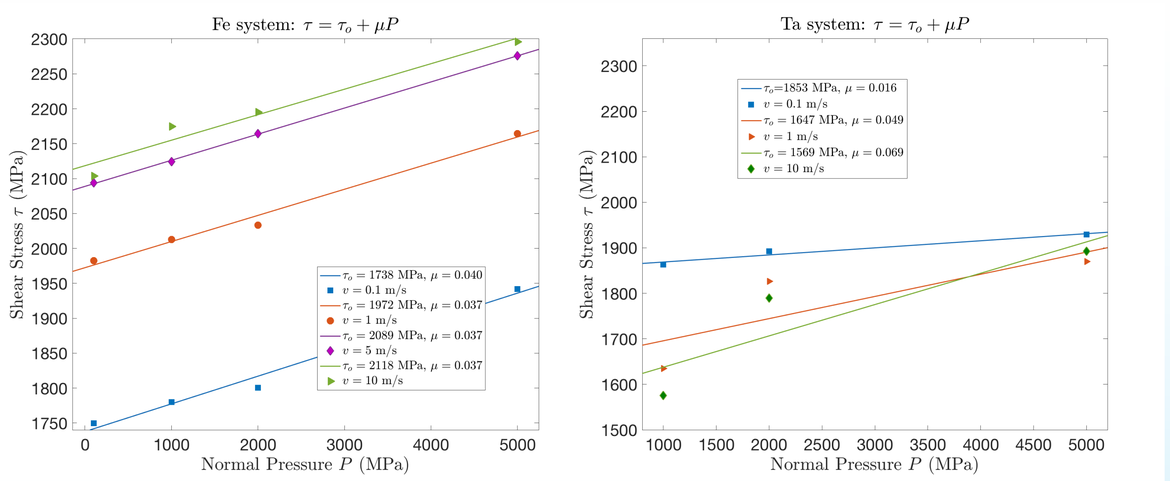
The average velocity of the atoms (left) in the sliding direction as function of the perpendicular dimension evolves from a linear profile to a nearly constant value. The initially linear profile reflects the prescribed sliding velocity applied to a thin layer of atoms at the very top of the system, and also reflects the thin layer at the very bottom slab which is held fixed. The system however quickly transitions to a state of nearly rigid-body sliding taking place at the bottom interface. The smaller grains which initially grow, stabilize once rigid-body sliding is reached. The velocity profiles for the Fe system at times $t < 10$ ns, unlike those for the Ta system, correspond to consistent trends in the friction behavior, namely that the friction force increases with increasing applied normal force.
The predominant carriers of plasticity in BCC metals are $\frac{1}{2}\langle 111\rangle$screw dislocations. This dislocation analysis (top right) indicates plastic deformation is initially mediated by intra-grain dislocation activity, which then transitions to grain-boundary sliding, a regime characteristic of very low friction. Under certain normal forces and sliding velocities, failure is observed at the interfaces (bottom right).





Related friction experiments in UHV of single crystalline Ta reveal that a low friction coefficient (left) can be achieved after a period of sliding. The friction map (right) shows the effect of different stresses on μ and delineates two distinct regimes separated by a limiting stress $\sigma = \sigma_y/\sqrt{3} = H/3\sqrt{3}$, the Tabor limit. Below this limit low friction is observed, while above the limit high friction and significant wear (plowing) ensue. In polycrystalline Ta however, which is much harder, the Tabor limit is far higher than the Hall-Petch limit and a wider range of intermediate friction behavior is possible. In single crystalline Ta the Tabor limit is still below the Beilby limit.





Friction can be described by a shear stress τ acting over a real contact area under an applied normal pressure P by

$$\tau = \tau_o + \mu P$$

where μ is the friction coefficient. Here τ_o is an intrinsic shear strength related to adhesion which becomes significant at the nanoscale. These preliminary MD calculations (left) show a trend in the friction behavior for the Fe system that is reflected in the sliding-velocity dependence, as well as a constant μ similar in value to what has been observed in FCC studies where very low friction occurs mediated primarily by grain-boundary sliding.

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