Sliding Over a Phase Transition*

Andrea Benassi
CNR-IOM Trieste and CNR-IENI Milano

*A. Benassi, A. Vanossi, G.L. Santoro and E. Tosatti PRL 106 256102 (2011)
A phase transition to control friction

Lubrication:
✓ Additives
✓ Organic molecule
✓ Bio molecules

Surface modification:
✓ Texturing
✓ Functionalization
✓ Coating (SEM,DLC,...)

Mechanical Vibrations
A phase transition to control friction

- The sliding bodies always play a passive role: we never exploit the material physical properties

- Dynamical control of friction: changing friction coefficient during sliding
A phase transition to control friction

Can we exploit the substrate physical properties to dynamically control friction?

We need a substrate with some tunable material property

Such a flexibility can be provided by the presence of a phase transition
Some experimental evidence

The effect of conductor/superconductor transition on dissipation and friction of...

... QCM adsorbates
Highland & Krim PRL (2006)

... pendulum type AFM
Kisiel et al.
Nature Mat. (2011)

FFM of TGS (Tc=49.9°C): the domain contrast disappears approaching Tc
Bluhm, Schwarz & Wiesendanger (1998)
Eng et al. (1999)

Friction force microscopy to image ferroelectric domains...

The presence of domains allows us to control the local value of the friction coefficient using temperature, electric fields or stress fields.
Our model experiment

The simplest case of structural phase transition is the **ferrodistortive** one: even if a distortion of the lattice cell take place, no net dipole moment arise and we can neglect all the electrostatic interactions.

Despite its simplicity, a model with an **inter-site potential** + a **multi well on-site potential** catch all the qualitative features of a structural phase transition.

We studied a 2D solid with a triangular lattice and an on-site potential with 6 wells in the directions of the nearest neighbors:

\[
U_{ij} = -U + \alpha (|r_i - r_j| - a)^2 + \beta (|r_i - r_j| - a)^4
\]

\[
U_i = U_M - \frac{2(U_M - U_m)}{a_0^2} \left( \frac{3x_i}{u_i} - 4\frac{x_i^3}{u_i^3} \right) u_i^2 + \frac{U_M - U_m}{a_0^4} u_i^4
\]

\( \mathbf{r} \) position vector \hspace{1cm} \( \mathbf{u} \) displacement vector
Close to the phase transition molecular dynamics simulations are strongly impaired by the critical slow-down: the fluctuations length-scale and time-scale diverge. However an estimation of the critical temperature can be given:

\[ C_V = \frac{1}{N_x N_z} \frac{\langle E^2 \rangle - \langle E \rangle^2}{K_B T^2} \]

\[ \chi_{yy} = -\frac{\langle y^2 \rangle - \langle y \rangle^2}{K_B T} \]

\[ \chi_{xx} = -\frac{\langle x^2 \rangle - \langle x \rangle^2}{K_B T} \]

We have a (quasi) second order phase transition with a critical temperature \( K T_c = 0.075 \) (LJ units)
The friction coefficient

- The friction force is non-monotonic, showing a maximum close to $T_c$.
- Below $T_c$ different polarizations give rise to very different friction force.
- This difference decreases and disappear moving closer to $T_c$.
- Increasing the vertical load the friction force becomes more sensitive to the different substrate polarizations.
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A peak at $T_c$ because of thermal activation friction is usually expected to decrease with temperature but thermal activation works on the substrate atoms too...

Increasing the temperature we open new dissipation channels helping the tip in kicking out the atoms from the well, and thus increasing the friction force.
A peak at Tc

Within the **linear response theory** (Ying et al. 1990-92), the damping coefficient relates to the microscopic properties of the substrate:

\[ \gamma = \frac{1}{K_B T} \sum_{ij} S_{ij} U(r - r_i^0) U(r - r_j^0) \]

\[ S_{ij} = F t [ < r_i(t) r_j(t') > ] \]

close to a **structural phase transition**, the correlation functions diverges, the viscous damping too and goes to zero.
Anisotropy below $T_c$

Being in different minima the substrate atoms experience a different slope of the on-site potential and this gives rise to a different resistance to the tip kicks.
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A model nano-brake

Acting with an external field we can exploit the friction coefficient difference below Tc to increase and decrease sliding friction.
Conclusion

The presence of a phase transition provides new degrees of freedom for the substrate physical properties

This degrees of freedom open up new dissipation channels for the slider/tip energy

Below Tc dissipation and friction can be controlled acting on this degrees of freedom with some external field

Model Improvements:
• Include dipole-dipole interaction (ferrodistortive to ferroelectric)
• Include electrostatic tip-substrate interaction and piezoelectric response
• Better tip description

Looking for different kinds of phase transition (ferromagnetic?)

Thanks for your attention!