Contact Mechanics and Elements of Tribology Lecture 3. Contact and Mechanics of Materials

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Surface properties:

- Friction
- Adhesion
- Wear

Surface properties are not fundamental

- Friction 🙁
- Adhesion [©]
- Wear 🙁

Surface properties are not fundamental

Friction 🙁

- Adhesion (2)
- Wear 🙁

Fundamental properties:

Volume:

- Young's modulus
- Poisson's ratio
- shear modulus
- yield stress
- mass density
- thermal properties

Surface properties are not fundamental

Friction 🙁

- Adhesion (2)
- Wear 🙁

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Surface:

- chemical reactivity
- absorbtion capabilities
- surface energy
- roughness

Surface properties are not fundamental

- Friction 🙁
- Adhesion ⁽²⁾
- Wear 🙁

Fundamental properties are interdependent

Volume:

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Surface properties are not fundamental

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- 🛛 Wear 🙁

More fundamental properties

- solids are made of atoms
- atoms are linked by bonds
- most of the volume and surface properties are the properties of the bonds

Fundamental properties are interdependent

Volume:

- Young's modulus
- Poisson's ratio
- shear modulus
- yield stress
- mass density
- thermal properties

Surface:

- chemical reactivity
- absorbtion capabilities
- surface energy
- roughness

Let's use atoms to simulate contacts

Let's start from the bottom

- Use Molecular Dynamics
- Potential for interaction between particles
- Time integration of the system evolution
- Natural coupling between thermal and mechanical phenomena
- Inherent platicity (dislocation movement)



Impact of a perfect crystal by a circular projectile



Impact of a perfect crystal by a circular projectile



Impact of a perfect crystal by a circular projectile: $20\,000$ particles on $20\,000$ time steps.



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Unfortunately it is hard to obtain valuable results at macroscopic scale using MD...

- How to get rid of the inherent adhesion between two surfaces?
- Hard to scale roughness to representative scale
- Too huge 3D simulations even for nano-indentation

Plasticity

Onset of plastic yielding

Hertz contact: body of revolution

Onset of plasticity for pressure

 $p_Y = 1.6\sigma_Y$

Associated force

 $F_Y = \frac{1.6^3 \pi^3 R^2}{6} \left(\frac{\sigma_Y}{E^*}\right)^2 \sigma_Y$

Associated contact radius

$$a_Y = \frac{1.6\pi R}{2} \frac{\sigma_Y}{E^*}$$

Plastic flow starts at depth

$$z_Y \approx 1.21 R \frac{\sigma_Y}{E^*}$$























Case: $\sigma_Y / E = 0.0005$





Evolution of the plastic zone in a sinusoidal asperity in contact with a rigid flat

Elastic-plastic normal contact: hardness

- Hardness ~ saturated plastic contact
- Recall: Vickers hardness HV = N/A
- Similarity solution^[1]

$$\frac{N}{\pi a^2 \sigma_Y} = F\left(\frac{a}{R}\frac{E}{\sigma_y}\right)$$

• Hardness $H \approx 3\sigma_Y$

 Hill R., Storøakers B., Zdunek A.B. A theoretical study of the Brinell hardness test. Proc R Soc Lond A 436 (1989)



solid with power-law hardening^[2]

Mesarovic S., N. Fleck, Spherical Indentation of Elastic-Plastic Solids, Proc R Soc Lond A 455 (1999)



Elasto-plastic contact under cyclic load









Deformation in fully plastic regime

✓ Mesh effect



Edge effect



[1] V. A. Yastrebov, J. Durand, H. Proudhon, G. Cailletaud, CR Mecan, 339:473-490 (2011)

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Near-surface vs bulk deformation

Material aspects

- Cold worked surface + recrystallized: smaller grains near the surface, Hall-Petch effect
- Thin coating films: nanograined, confined plasticity, Hall-Petch effect
- Oxides: brittle hard films

Geometrical aspects

- Roughness of all nature
- Indentation by asperities: confined plastic zone, high plastic strain gradients


Onset of yielding at atomic scale







[1] Nix, Gao. J Mech Phys Solids (1998).



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 Feng, Nix. Scripta Mater (2004).



[1] Nix, Gao. J Mech Phys Solids (1998).

[2] Feng, Nix. Scripta Mater (2004).

[3] Qui, Huang, Nix, Hwang, Gao. Acta Mater (2001).



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Nix, Gao. J Mech Phys Solids (1998).
 Feng, Nix. Scripta Mater (2004).
 Qui, Huang, Nix, Hwang, Gao. Acta Mater (2001).

[4] Swadener, George, Pharr. J Mech Phys Solids (2002).
[5] Gao, Larson, Lee, Nicola, Tischler, Pharr. J Appl Mech (2015).

- Crystal plasticity models in indentation all slip systems are activated
 Difference with isotropic plasticity is small
- Discrete models with inherent characteristic length
 - Molecular Dynamics -Dislocation Dynamics
- Continuum models with characteristic length
 - Cosserat continuum^[1]
 - Second-gradient plasticity^[2]

 Forest S., Sievert R. Elastoviscoplastic constitutive frameworks for generalized continua. Acta Mech 160 (2003)

[2] Cordero N.M., Forest S. et al. Grain size effects on plastic strain and dislocation density tensor fields in metal polycrystals, Comp Mater Sci 52 (2012)



Spherical indentation of FCC copper crystal using crystal plasticity model in Zset

Casals O., Forest S. Finite element crystal plasticity analysis of spherical indentation in bulk single crystals and coatings. Comp Mater Sci 45 (2009)

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MD simulation of a spherical indentation on (111) FCC cube

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Resulting DD simulation of a spherical indentation on (111) FCC cube

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DD simulation of Berkovich nanoindentation

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www.numodis.com

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Cosserat continuum

- Field variables (displacement & rotation): <u>u</u>, <u>w</u>
- Small deformation tensor: $\underline{\underline{\varepsilon}} = \nabla \underline{u} + {}^{3}\underline{\underline{\varepsilon}} \cdot \underline{\omega}$
- Torsion-curvature tensor: $\underline{\kappa} = \nabla \underline{\omega}$
- $= \text{ Elasticity: } \underline{\sigma} = \lambda \operatorname{tr}\left(\underline{\underline{\varepsilon}}_{e}\right) \underline{I} + \mu(\underline{\underline{\varepsilon}}_{e} + \underline{\underline{\varepsilon}}_{e}^{\mathsf{T}}) + \mu_{c}(\underline{\underline{\varepsilon}}_{e} \underline{\underline{\varepsilon}}_{e}^{\mathsf{T}}), \quad \underline{\underline{m}} = \alpha \operatorname{tr}\left(\underline{\underline{\kappa}}_{e}\right) \underline{I} + 2\beta \underline{\underline{\kappa}}_{e} \\ \boxed{l_{e} = \sqrt{\beta/\mu}}$

Note: $\underline{\underline{\varepsilon}}^{\mathsf{T}} \neq \underline{\underline{\varepsilon}}, \underline{\underline{\kappa}}^{\mathsf{T}} \neq \underline{\underline{\kappa}}, \underline{\underline{\sigma}}^{\mathsf{T}} \neq \underline{\underline{\sigma}}, \underline{\underline{m}}^{\mathsf{T}} \neq \underline{\underline{m}}$

In non-inertial problems without volume forces and couple-forces, balance of momentum and of moment of momentum:

 $\nabla \cdot \underline{\sigma} = 0, \quad \nabla \cdot \underline{m} - {}^{3}\underline{\epsilon} : \underline{\sigma} = 0$

- Plasticity: equivalent stress^[1,2] $Y = \sqrt{\frac{3}{2}} \left(a_1 \underline{s} : \underline{s} + a_2 \underline{s} : \underline{s}^{\mathsf{T}} + \left| \frac{1}{l_n^2} \right| \underline{m} : \underline{m} \right)$
- Internal lengths: elastic *l_e*, plastic *l_p*

R. de Borst, L.J. Sluys, Comp Meth Appl Mech Engin (1991)
 S. Forest, R. Sievert, Acta Mech (2003)

where permutation tensor ${}^{3}\underline{e} \sim \epsilon_{ijk} = \begin{cases} 1, & \text{if } \{ijk\} = \{123\} \text{ or } \{231\} \text{ or } \{312\} \\ -1, & \text{if } \{ijk\} = \{321\} \text{ or } \{213\} \text{ or } \{132\} \\ 0, & \text{otherwise} \end{cases}$ V.A. Yastrebov Lecture 3 49/112

Single asperity analysis

Assumptions

- Rigid spherical asperity
- Axisymmetric FE problem
- Generalized Cosserat continuum

Parameters

- Au: E = 96 GPa, ν = 0.42, σ_y = 140 MPa
- $\mu_c = 10\mu, l_e = 100 \text{ nm}, a_1 = 1$
- Indenter radius $R \in [0.002, 2000] \ \mu m$

Objectives

- Study size effect
- Enhance asperity based models for rough contact



Accumulated plasticity

• Different plastic distribution



Indenter radius $R = 20 \mu m$ Max plastic strain $p_{max} \approx 7.5\%$ Indenter radius $R = 2\mu m$ Max plastic strain $p_{max} \approx 11\%$

Displacement-force-contact radius



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Viscoelasticity

Viscoelastic material

One-dimensional constitutive equations

- Applied stress σ
- In the left branch $\sigma_1 = E_{\infty}\varepsilon$
- In the dashpot $\sigma_2 = \eta \dot{\varepsilon}_d$ (*)
- In the right spring $\sigma_2 = E(\varepsilon \varepsilon_d)$ (**)
- For the whole system $\sigma = \sigma_1 + \sigma_2$

$$\sigma = (E_{\infty} + E)\varepsilon - E\boldsymbol{\varepsilon_d}$$

From (*) and (**), and denoting $\tau = \eta/E$:

$$\boxed{\frac{\dot{\varepsilon}_d}{\tau} + \frac{\varepsilon_d}{\tau} = \frac{\varepsilon}{\tau}}, \quad \varepsilon_d \xrightarrow[t \to -\infty]{} 0$$



One-dimensional viscoelastic model

Recall: 1D model

$$\sigma = (E_{\infty} + E)\varepsilon - E\varepsilon_d, \quad \dot{\varepsilon}_d + \frac{\varepsilon_d}{\tau} = \frac{\varepsilon}{\tau}, \quad \varepsilon_d \xrightarrow[t \to -\infty]{} 0$$

Multiple dashpots in parallel

$$\sigma = (E_{\infty} + \sum_{i} E_{i})\varepsilon - \sum_{i} E_{i}\varepsilon_{d}^{i}, \quad \dot{\varepsilon}_{d}^{i} + \frac{\varepsilon_{d}^{i}}{\tau_{i}} = \frac{\varepsilon}{\tau_{i}}, \quad \varepsilon_{d}^{i} \xrightarrow[t \to -\infty]{} 0, \quad \tau_{i} = \frac{\eta_{i}}{E_{i}}$$

elastic stress σ_0



One-dimensional viscoelastic model

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Multiple dashpots in parallel

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elastic stress σ_0

• Denote $E_0 = E_{\infty} + \sum_i E_i$, $\psi_i = E_i/E_0$, and $q_i = E_i \varepsilon_d^i$ we obtain

$$\sigma = E_0 \varepsilon - \sum_i q_i, \quad \dot{q}_i + \frac{q_i}{\tau_i} = \frac{\psi_i}{\tau_i} \sigma_0, \quad \varepsilon_d^i \xrightarrow[t \to -\infty]{} 0$$

By construction

$$\sum_{i} \psi_{i} + \frac{E_{\infty}}{E_{0}} = 1 \quad \Rightarrow \quad \sum_{i} \psi_{i} = 1 - \frac{E_{\infty}}{E_{0}}$$

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• Three-dimensional viscoelastic model

Linear viscoelastic (generalized Maxwell model, standard solid)

Stress-strain relation:

$$\underline{\underline{\sigma}}(t) = K\theta \underline{\underline{I}} + \int_{-\infty}^{\tau} G(t-\tau) \underline{\underline{\dot{e}}}(\tau) d\tau,$$

• Kernel $G(\tau)$ is given by:

 $G(\tau) = 2G_{\infty} + 2(G_0 - G_{\infty})\Psi(\tau) \text{ with } \Psi(\tau) = \sum_{i=1}^n \psi_i \exp(-\tau/\tau_i)$

- G_∞, G₀ are the slow/fast loading shear moduli, respectively, such that G_∞ ≤ G₀;
- *K* is the bulk modulus, and for elastomers/polymers $K/G_0 \gg 1$;
- ψ_i are the influence coefficients, such that $\sum_{i=1}^{n} \psi_i = 1$;
- τ_i are the respective relaxation times.

• Material model: *storage* and loss moduli

- Consider a harmonic (rigid) loading: $\underline{e}(t) = \underline{e}_0 \exp(i\omega t)$
- Split the kernel: $G(t) = 2G_{\infty} + \tilde{G}(t)$
- Then, the storage modulus (general case):

$$G'(\omega) = 2G_{\infty} + \omega \int_{0}^{\infty} \tilde{G}(\tau) \sin(\omega\tau) d\tau$$

The storage modulus in the framework of the generalized Maxwell model:

$$G'(\omega) = 2G_{\infty} + 2\omega(G_0 - G_{\infty})\sum_{i=1}^n \psi_i \int_0^\infty \exp(-\tau/\tau_i)\sin(\omega\tau)\,d\tau$$
$$G'(\omega) = 2G_{\infty} + 2(G_0 - G_{\infty})\sum_{i=1}^n \frac{\psi_i \omega^2 \tau_i^2}{1 + \omega^2 \tau_i^2}$$

Remark:

•

$$\int \exp(cx)\sin(bx)\,dx = \frac{\exp(cx)}{c^2 + b^2}[c\sin(bx) - b\cos(bx)]$$

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• Material model: storage and *loss* moduli

The loss modulus (general case):

$$G''(\omega) = \omega \int_{0}^{\infty} \tilde{G}(\tau) \cos(\omega \tau) d\tau$$

The loss modulus in the framework of the generalized Maxwell model:

$$G''(\omega) = 2\omega(G_0 - G_\infty) \sum_{i=1}^n \psi_i \int_0^\infty \exp(-\tau/\tau_i) \cos(\omega\tau) d\tau$$
$$G''(\omega) = 2(G_0 - G_\infty) \sum_{i=1}^n \frac{\psi_i \omega \tau_i}{1 + \omega^2 \tau_i^2}.$$

Remark:

$$\int \exp(cx)\cos(bx)\,dx = \frac{\exp(cx)}{c^2 + b^2}[c\cos(bx) + b\sin(bx)]$$

- Material parameters: $G_0 = 1.1$ MPa, $G_{\infty} = 50$ kPa
- Single relaxation time: $\tau_0 = 10^{-7} \text{ s}$
- Quasi-incompressible material: $K/G_0 = 10^6 \gg 1$
- Uniaxial (rigid) loading: $\varepsilon_{xx} = A \sin(\omega t)$, $\sigma_{yy} = \sigma_{zz} = 0$, $\varepsilon_{yy} = \varepsilon_{zz} \approx -0.5\varepsilon_{xx}$
- Spherical and deviatoric parts: $\underline{e} \approx A(1-2\nu)\sin(\omega t)\underline{I}, \underline{e} \approx \underline{e}$
- Stress-strain relation:

$$\underline{\sigma}(t) = \int_{-\infty} 2(G_0 - G_\infty) \exp[-(t - \tau)/\tau_0] \underline{\dot{e}}(\tau) d\tau + 2G_\infty \underline{e} + K\underline{e},$$

Axial and radial stress components:

$$\sigma_{xx} = 2G_{\infty}\varepsilon_{xx} + K(\varepsilon_{xx} + 2\varepsilon_{yy}) + \int_{-\infty}^{t} 2(G_0 - G_{\infty}) \exp[-(t - \tau)/\tau_0]\dot{\varepsilon}_{xx}(\tau)d\tau$$

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 $\sigma_{yy}=0$

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$$\sigma_{xx} = 3G_{\infty}\varepsilon_{xx} + \int_{-\infty}^{t} 3(G_0 - G_{\infty}) \exp[-(t - \tau)/\tau_0]\dot{\varepsilon}_{xx}(\tau)d\tau$$

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Uniaxial storage modulus:

$$E'(\omega) = 3G_{\infty} + 3(G_0 - G_{\infty})\frac{\omega^2 \tau_0^2}{1 + \omega^2 \tau_0^2}$$

Uniaxial loss modulus:

$$E''(\omega) = \mathbf{3}(G_0 - G_\infty) \frac{\omega \tau}{1 + \omega^2 \tau_0^2}$$







Linear frequency $f = 10^4 \text{ Hz}$





Linear frequency $f = 10^6 \text{ Hz}$



Linear frequency $f = 10^7 \text{ Hz}$



Linear frequency $f = 10^8 \text{ Hz}$

Viscoelastic sliding: bulk friction








 $T = 120 \ ^{\circ}\text{C}$



Simulation sketch



Effect of bringing-in-contact rate on frictional force evolution

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Material properties interdependence



Rabinowicz, Friction and wear of materials, Wiley (1965)

Material properties interdependence



Rabinowicz, Friction and wear of materials, Wiley (1965)

Material properties interdependence



Thermal coefficient of expansion and Young's modulus interdependence

Rabinowicz, Friction and wear of materials, Wiley (1965)



Surface energy and hardness interdependence

Real area of contact depends on

Real area of contact depends on

normal load:

real area of contact is proportional to the normal load and inversely proportional to the hardness H



 A_r - real contact area, p_0 - applied pressure

Real area of contact depends on

normal load:

real area of contact is proportional to the normal load and inversely proportional to the hardness H

$$A_r = A_0 \frac{p_0}{H}$$

 A_r - real contact area, p_0 applied pressure; H hardness, A_0 - nominal contact area

Real area of contact depends on

normal load:

real area of contact is proportional to the normal load and inversely proportional to the hardness H

sliding distance:

contact area might be significantly smaller than before shear forces were first applied



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time:

real area of contact increases with time (for creeping materials)



Sliding distance

Real area of contact depends on

normal load:

real area of contact is proportional to the normal load and inversely proportional to the hardness H

sliding distance:

contact area might be significantly smaller than before shear forces were first applied

time:

real area of contact increases with time (*for creeping materials*)

surface energy:

the higher the surface energy, the greater the area of contact



Engineering friction

First approximations: friction coefficient does not depend on

- normal load
- apparent area of contact
- velocity
- surface roughness
- repose time
- friction force direction is opposite to the sliding

Engineering friction

First approximations: friction coefficient does not depend on

- normal load ☺/☺
- apparent area of contact ☺
- velocity 🙁
- surface roughness ☺/☺
- repose time 🙁/☺
- friction force direction is opposite to the sliding (2)

First approximation: **Exceptions**:

 friction coefficient does not depend on normal load.

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 friction coefficient does not depend on normal load.



Rabinowicz, Friction and wear of materials, Wiley (1965)

Exceptions:

at micro scale for small slidings

First approximation:

 friction coefficient does not depend on normal load.



Rabinowicz, Friction and wear of materials, Wiley (1965)

- at micro scale for small slidings
- for huge pressures (metal forming) friction force is limited

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 friction coefficient does not depend on normal load.



 Rabinowicz, Friction and wear of materials, Wiley (1965)

- at micro scale for small slidings
- for huge pressures (metal forming) friction force is limited
- for too hard (diamond) or too soft (teflon) materials:

• generally
$$T = cF^{\alpha}, \alpha \in \left[\frac{2}{3}; 1\right];$$

First approximation:

 friction coefficient does not depend on normal load.



Rabinowicz, Friction and wear of materials, Wiley (1965)

Exceptions:

- at micro scale for small slidings
- for huge pressures (metal forming) friction force is limited
- for too hard (diamond) or too soft (teflon) materials:

generally
$$T = cF^{\alpha}, \alpha \in \left[\frac{2}{3}; 1\right];$$

hard coating (film) and a softer substrate





Real friction :: normal force



Courtney-Pratt J. S., and E. Eisner. The effect of a tangential force on the contact of metallic bodies. Proc R Soc A 238 (1957)

Real friction :: normal force



First approximation:

 friction force direction is opposite to the sliding.

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Exceptions:

 the direction of the friction force remains within [178; 182] degrees to sliding direction (fig. 1);



Direction of friction force in sliding

[1] Rabinowicz, Friction and wear of materials, Wiley (1965)

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- the difference is higher for anisotropic surface roughness



Direction of friction force in sliding

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First approximation:

 friction force direction is opposite to the sliding.

- the direction of the friction force remains within [178; 182] degrees to sliding direction (fig. 1);
- the difference is higher for anisotropic surface roughness
- asymmetry of roughness and friction



Examples of asymmetric friction

Real friction :: apparent area and roughness

First approximation:

 Friction coefficient does not depend on the apparent area of contact

Exceptions:

First approximation:

 Friction coefficient does not depend on surface roughness

Real friction :: apparent area and roughness

First approximation:

 Friction coefficient does not depend on the apparent area of contact

Exceptions:

very smooth and clean surfaces

First approximation:

 Friction coefficient does not depend on surface roughness

Real friction :: apparent area and roughness

First approximation:

 Friction coefficient does not depend on the apparent area of contact

Exceptions:

very smooth and clean surfaces

First approximation:

 Friction coefficient does not depend on surface roughness

Exceptions:

too smooth or too rough surfaces



Effect of roughness on the coefficient of friction

[1] Rabinowicz, Friction and wear of materials, Wiley (1965)

Real friction :: time and velocity

First approximation:

 Friction coefficient does not depend on time

Exceptions:

First approximation:

 Friction coefficient does not depend on sliding velocity

Real friction :: time and velocity

First approximation:

 Friction coefficient does not depend on time

Exceptions:

creeping materials

First approximation:

 Friction coefficient does not depend on sliding velocity

Exceptions:

Static friction
$$f_s = f_0 + kt^{1/10}$$

Time of stick, t

Evolution of the static coefficient of friction with the time of repose

Real friction :: time and velocity

First approximation:

 Friction coefficient does not depend on time

Exceptions:

creeping materials



First approximation:

 Friction coefficient does not depend on sliding velocity

Exceptions:

 if material behaves differently at different loading rate, then the friction depends on the sliding velocity



Sliding speed, v

Evolution of the static coefficient of friction with the time of repose

Kinetic friction decreases with increasing sliding velosity

V.A. Yastrebov

Lecture 3

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Real friction :: velocity

First approximation:

 Friction coefficient does not depend on sliding velocity

- if material behaves differently at different loading rate (polymers)
- considerable rise in temperature (thermo-mechanical coupling)
Real friction :: velocity



Friction coefficient slightly decreses with increasing velocity of sliding, titanium on titanium

First approximation:

 Friction coefficient does not depend on sliding velocity

Exceptions:

- if material behaves differently at different loading rate (polymers)
- considerable rise in temperature (thermo-mechanical coupling)

Real friction :: velocity



Friction coefficient slightly decreses with increasing velocity of sliding, titanium on titanium

First approximation:

 Friction coefficient does not depend on sliding velocity

Exceptions:

- if material behaves differently at different loading rate (polymers)
- considerable rise in temperature (thermo-mechanical coupling)



Friction coefficient dependence on velocity of sliding for lubricated surfaces

Real friction :: velocity



Friction coefficient increases and decreases with increasing velocity of sliding, hard on soft (steel on lead, steel on indium)

First approximation:

 Friction coefficient does not depend on sliding velocity

Exceptions:

- if material behaves differently at different loading rate (polymers)
- considerable rise in temperature (thermo-mechanical coupling)



Friction coefficient dependence on velocity of sliding for lubricated surfaces

Thank you for your attention!