

微纳结构材料力学行为中的表/ 界面效应模拟

黄干云

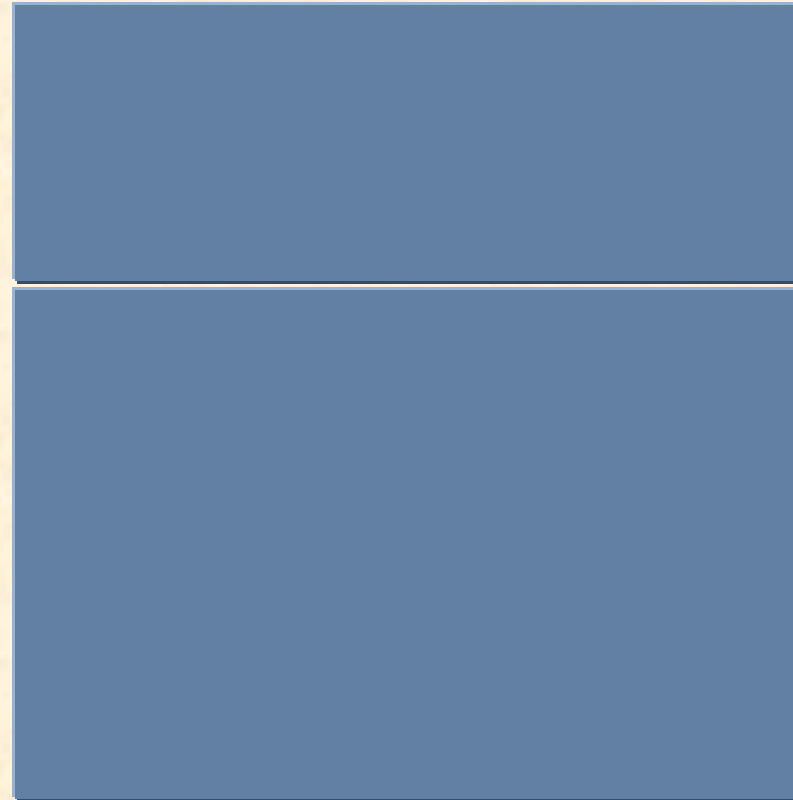
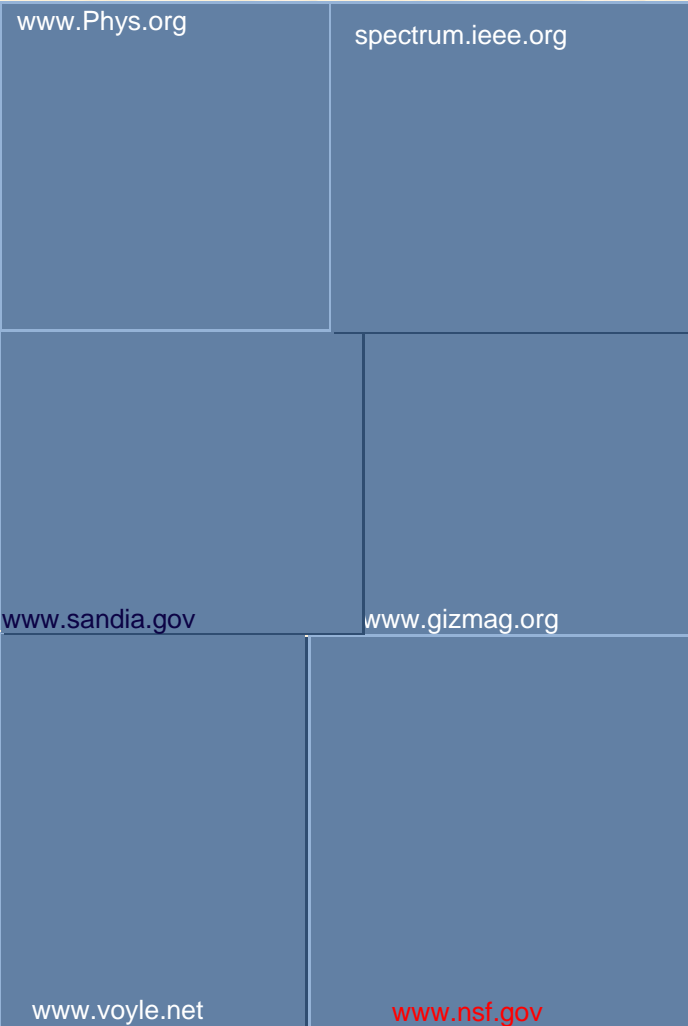
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主要内容

- 背景
- 纳米结构材料弹性行为的表面弹性模拟
- 考虑表/界面能影响的位错-表/界面相互作用
- 考虑表/界面效应的连续分布位错晶体塑性模型

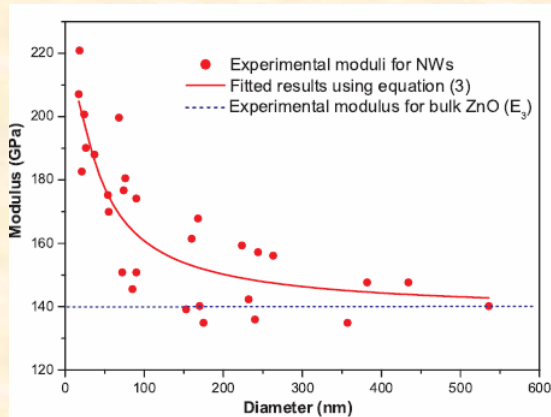
背景



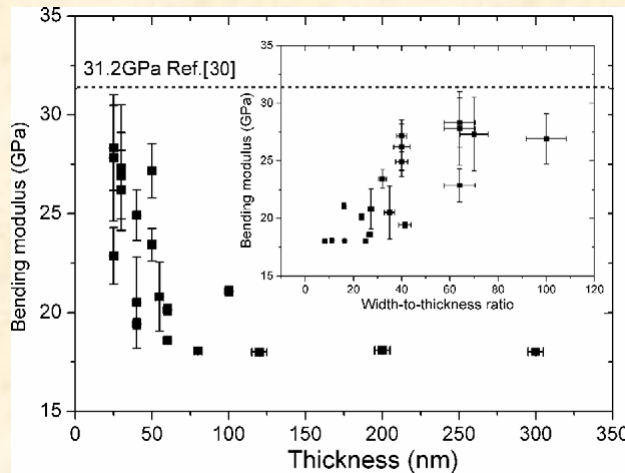
Daoud and Xin Chem Commun. 2005, 2110-2112
Podsiadlo et al. Science, 2007,318,80-83

纳米结构弹性性质的尺寸效应

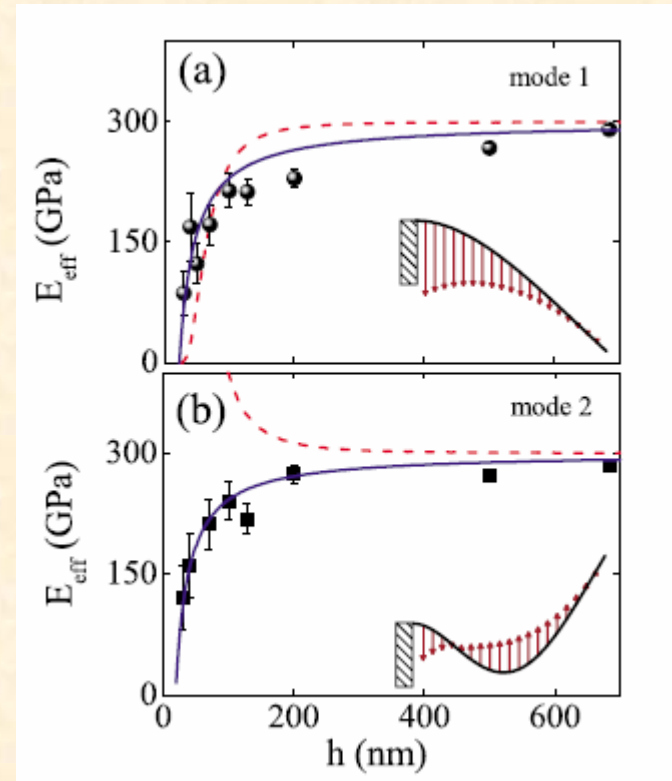
Size dependent moduli of nanostructures



ZnO nanowire [Chen et al. PRL 96, 075505, 2006]



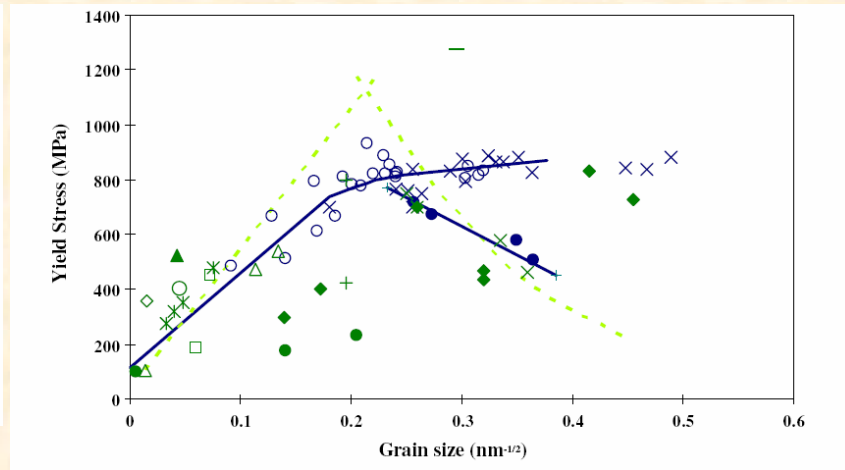
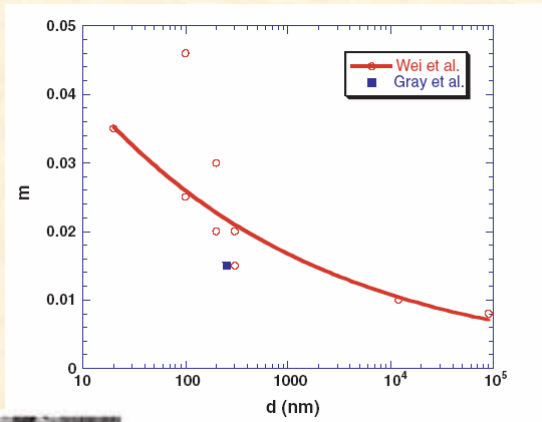
BN Nanosheet [Li et al. Nanotechnology 20, 385707, 2009]



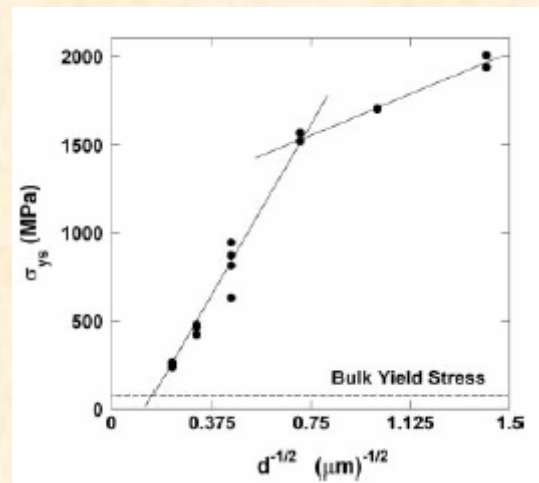
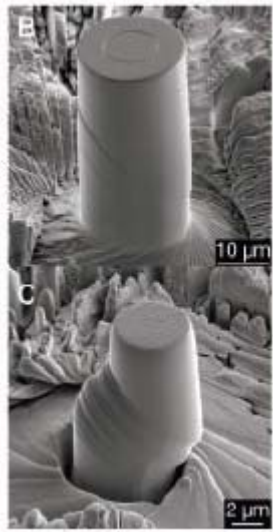
SN cantilever [Gavan et al. APL 94, 233108, 2009]

- Surface/interface effect
- Nonlocal effect
- Gradient effect

纳米晶体材料塑性行为的尺寸效应



Meyer et al. Prog Mater. Sci., 51, 427-556, 2006



- Surface/interface effect
- Strain gradient effect

Uchic et al. Science, 305, 986-989, 2004

从考虑表/界面能的角度, 就力学行为中的表/
界面效应模拟展开了一点工作

纳米结构材料弹性行为的表面弹性模拟

- Gurtin and Murdoch (Arch Rat Mech Anal. 57, 291-323, 1975), Cammarata (prog. Surf. Sci. 46, 1-38, 1994), Miller and Shenoy (Nanotechnology, 11, 139-147, 2000)

$$\sigma_{\alpha\beta}^s = \gamma\delta_{\alpha\beta} + \frac{\partial\gamma}{\partial\varepsilon_{\alpha\beta}} \text{ or } = \sigma_{\alpha\beta}^{s0} + c_{\alpha\beta\chi\gamma}^s \varepsilon_{\chi\gamma}$$

Boundary conditions

$$\sigma_{\alpha\beta,\beta}^s + t_\alpha = 0, \quad \sigma_{\alpha\beta}^s \kappa_{\alpha\beta} = \sigma_{ij} n_i n_j$$

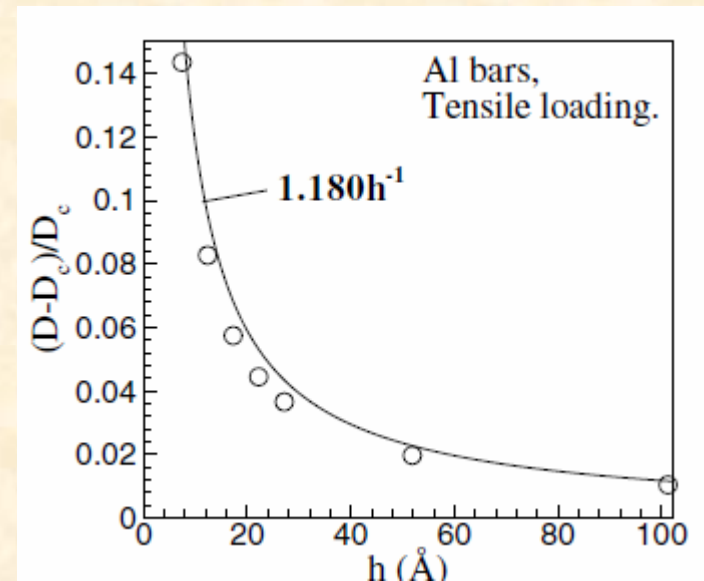
t_α the component of $\sigma_{ij} n_j$ along α direction

$\kappa_{\alpha\beta}$ curvature tensor.

Duan et al (JMPS, 2005), He et al, (IJSS, 2004)

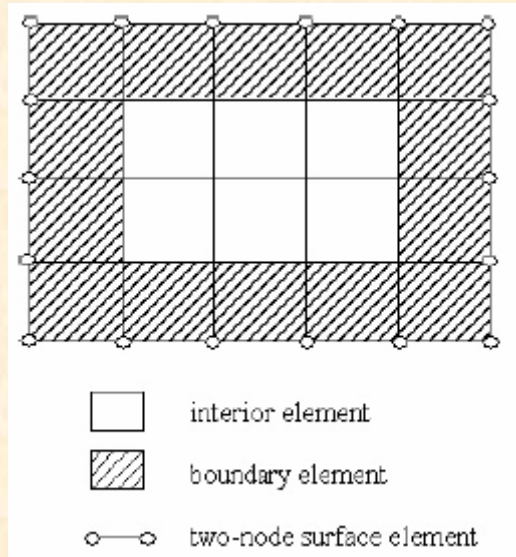
Wang (APL, 2007) and Wang et al (EPL, 2007)

.....



Miller & Shenoy, Nanotechnology,
11, 139-147, 2000

Finite element method by accounting for surface elasticity (Gao et al, Nanotechnology, 17, 1118-22, 2006)



$$U^s = \frac{1}{2} \iint_A \{\delta_e\}^T [K_e^s] \{\delta_e\} dA + \iint_A \{\delta_e\}^T \{P_e^s\} dA$$

$$[K_e^s] = [B]_{surf}^T [K_e^s] [B]_{surf}$$

$$\{P_e^s\} = [B]_{surf}^T \{F\}$$

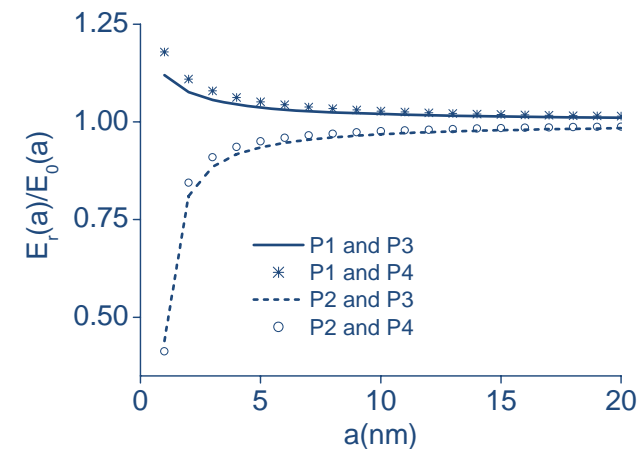
$[K_e] \{\delta_e\} = \{P_e\}$ for elements in the bulk

$[[K_e] + [K_e^s]] \{\delta_e\} = \{P_e\} - \{P_e^s\}$ for elements on the surface

Surface piezoelectricity (Huang and Yu, Phys. Stat. Solids B, 243, R22-24, 2006)

$$\Gamma(\varepsilon_{\alpha\beta}, E_\alpha) = \Gamma_0 + \sigma_{\alpha\beta}^{s0} \varepsilon_{\alpha\beta} + \frac{1}{2} c_{\alpha\beta\gamma\gamma}^s \varepsilon_{\alpha\beta} \varepsilon_{\gamma\gamma} + D_i^{s0} E_i + \frac{1}{2} \kappa_{ij}^s E_i E_j + e_{\alpha\beta j}^s \varepsilon_{\alpha\beta} E_j$$

$$\sigma_{\alpha\beta}^s = \sigma_{\alpha\beta}^{s0} + c_{\alpha\beta\gamma\gamma}^s \varepsilon_{\gamma\gamma} + e_{\alpha\beta j}^s E_j, \quad D_i^s = D_i^{s0} + \kappa_{ij}^s E_j + e_{\alpha\beta j}^s \varepsilon_{\alpha\beta}$$



压电圆环内径处的电场强度

Surface Green's functions with account of surface elasticity (Huang and Yu, JApM 2007)

$$g_1 = -\frac{\exp[(ix_1 - x_3)/l]Ei[(-ix_1 + x_3)/l] + \exp[-(ix_1 + x_3)/l]Ei[(ix_1 + x_3)/l]}{2l}$$

$$g_2 = \frac{\exp[(ix_1 - x_3)/l]Ei[(-ix_1 + x_3)/l] - \exp[-(ix_1 + x_3)/l]Ei[(ix_1 + x_3)/l]}{2il}$$

$$u_{31}(x_1, x_3) = -\frac{1-2\nu}{2\pi\mu} \tan^{-1}(x_3/x_1) + \frac{1}{2\pi\mu} [l(1-2\nu) + x_3]g_2,$$

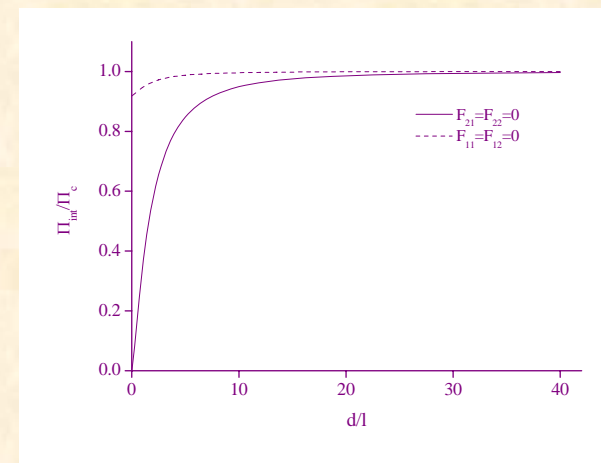
$$u_{13}(x_1, x_3) = \frac{1}{2\pi\mu} \left\{ (1-2\nu) \tan^{-1}\left(\frac{x_3}{x_1}\right) + \frac{1}{2(1-\nu)} \frac{x_1 x_3}{R^2} + (1-2\nu) \left[\frac{x_3}{2(1-\nu)} + l \right] g_2 \right\},$$

$$u_{33}(x_1, x_3) = -\frac{1}{2\pi\mu} \left\{ (1-\nu) \ln R^2 - \frac{1}{2(1-\nu)} \frac{x_3^2}{R^2} + \frac{1-2\nu}{2(1-\nu)} [x_3 + (1-2\nu)l] g_1 \right\}$$

$$u_{11}(x_1, x_3) = -\frac{1-\nu}{2\pi\mu} \ln R^2 + \frac{1}{2\pi\mu} [x_3 - 2(1-\nu)l] g_1,$$

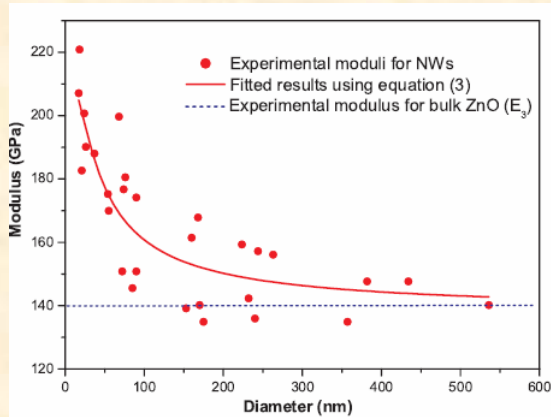
$$R^2 = x_1^2 + x_3^2$$

Effect of surface elasticity is notable within the range of several nanometers!

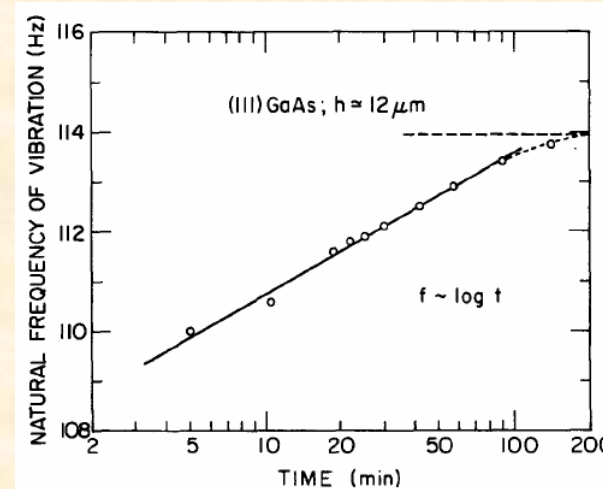


Elastic interaction between steps

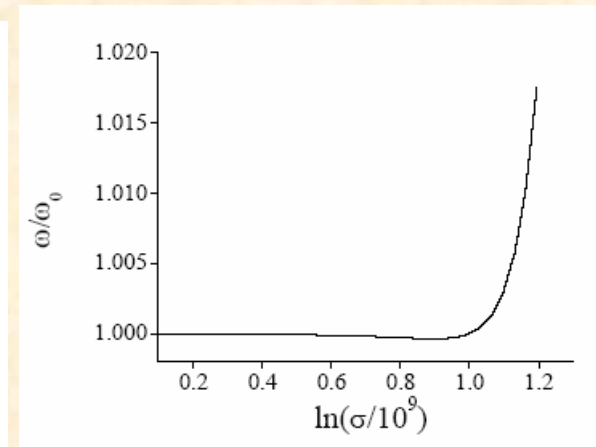
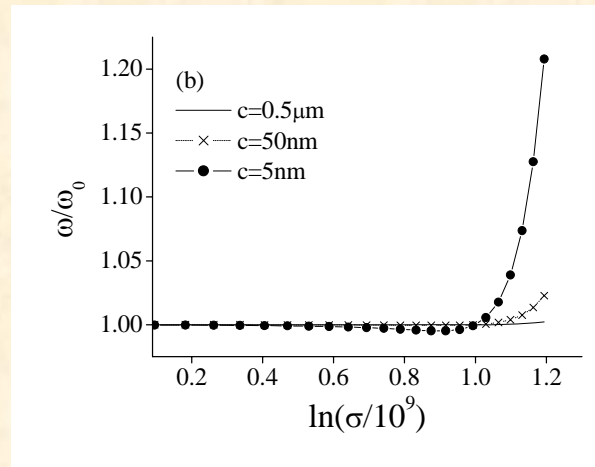
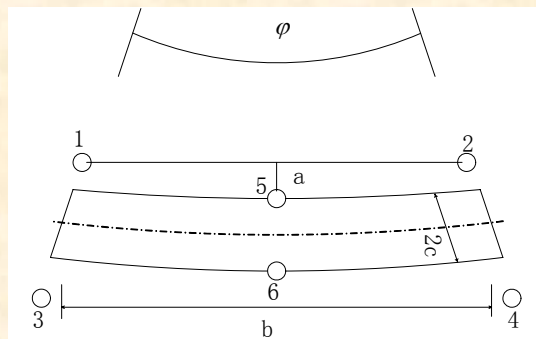
Effect of adsorption on the vibration of a cantilever



ZnO nanowire [Chen et al. PRL 96, 075505, 2006]



Lagowski et al., APL 26, 493-495, 1975



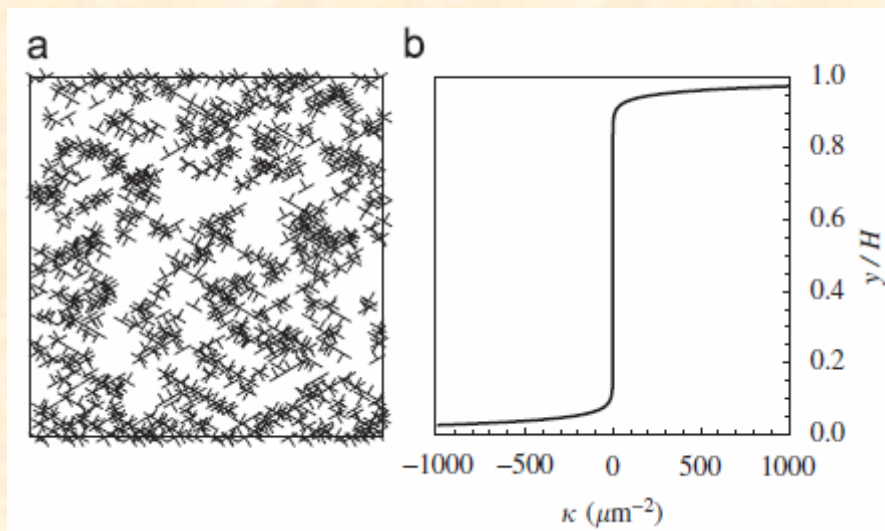
See Huang et al, APL, 89, 043506, 2006

Interaction between one dislocation and a surface/interface

In DDS (e.g., van der Giessen et al, JMPS, 2133-53, 2001) and DiFT (Limkumnerd and van der Giessen, JMPS, 3304-14,2008), dislocation motion is governed by the force acting on it

$$f = \tau b$$

f Peach-Koehler force, τ the resolved stress on the slip plane at the dislocation line; b the Burger's vector



Dislocations are densely distributed near the surface/interface! Influence of surface/interface energy?

Limkumnerd and van der Giessen, JMPS, 3304-14,2008

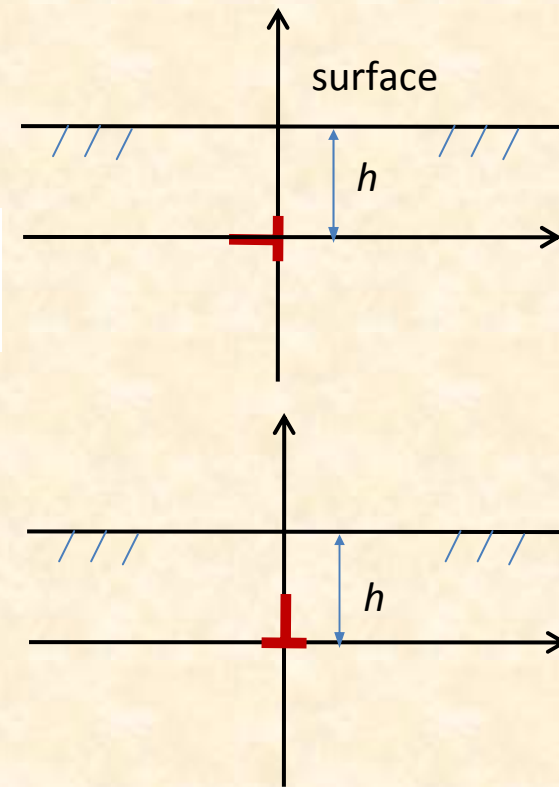
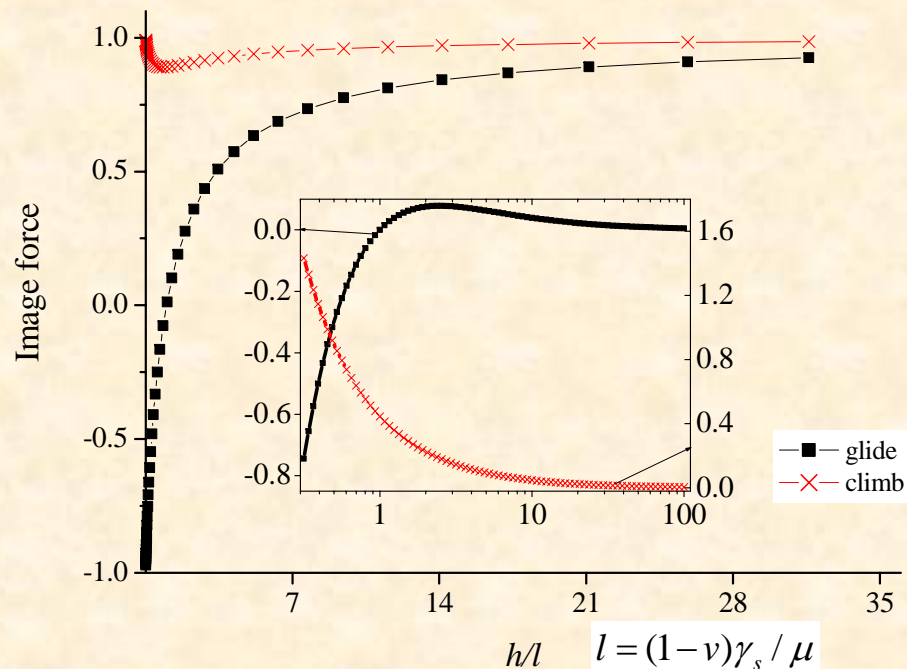
Effect of surface energy on the dislocation-surface interaction

Surface energy:
$$\int_A \gamma_s \sqrt{1+u_{2,1}^2} dx \approx \int_A \gamma_s (1+u_{2,1}^2 / 2) dx$$

Boundary conditions

$$\sigma_{22}(x_1, h) = \mu u_{2,11}, \sigma_{21}(x_1, h) = 0,$$

$$[u_2(x_1, 0)] = b_2 H(x_1), [u_1(x_1, h)] = b_1 H(x_1),$$



The image force on the dislocation can be repulsive!

Dislocation-grain boundary interaction by accounting for grain boundary energy

Grain boundary energy:

$$\int_A \gamma_{gb} \sqrt{1 + u_{2,1}^2} dx \approx \int_A \gamma_{gb} (1 + u_{2,1}^2 / 2) dx$$

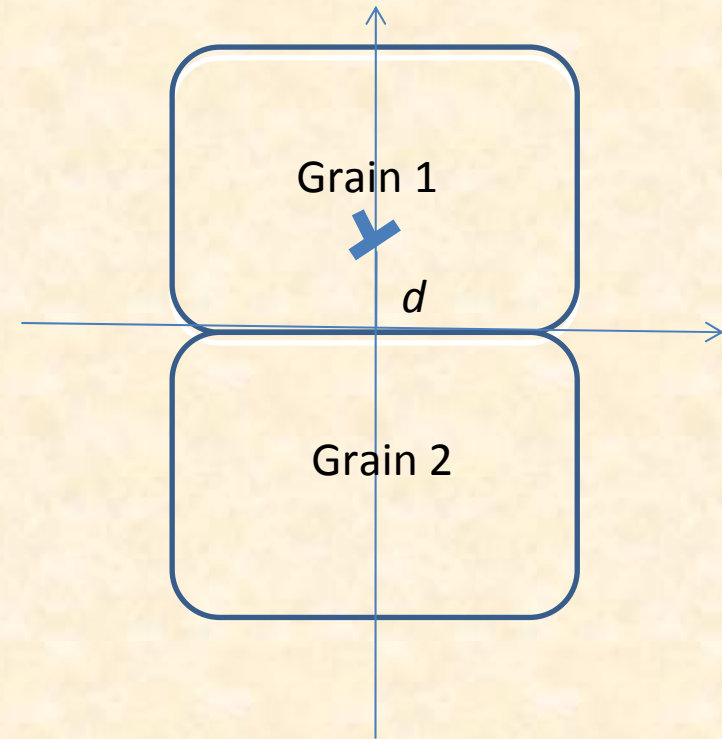
Bulk elastic energy:

$$U_e = \int_V \sigma_{ij} \varepsilon_{ij} / 2 dV$$

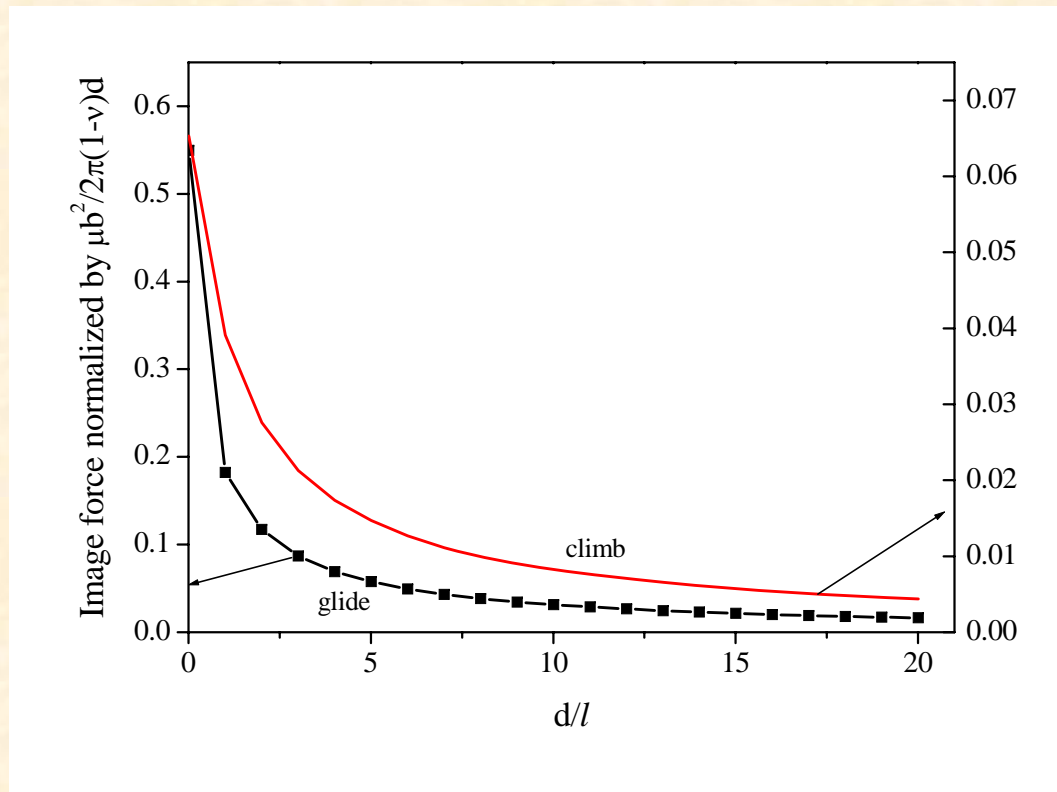
Boundary conditions:

$$[\sigma_{22}(x_1, 0)] = \mu_{2,11}, [\sigma_{21}(x_1, 0)] = 0, [u_2(x_1, 0)] = 0, [u_1(x_1, 0)] = 0,$$

$$[\sigma_{22}(x_1, d)] = 0, [\sigma_{21}(x_1, 0)] = 0, [u_2(x_1, 0)] = b_2 H(x_1), [u_1(x_1, 0)] = b_1 H(x_1),$$



No grain boundary sliding or de-cohesion!



What is the effect of grain boundary sliding?

What if the grains possess different elastic constants?

How will the image forces influence the plastic behavior of nano-crystalline materials?

Distributed dislocation model for crystal plasticity with account of surface/interface energy

-- Accounting for surface/interface energy

$$E_s = \int_{\partial V} \Gamma(\varepsilon_{ij}^e, \varepsilon_{ij}^p) dA$$

--Accounting for strain gradient effect (See the bulk energy density, Le and Sembrion, 2008)

$$U = U_{el} - \mu\eta \ln(1 - \rho/\rho_s)$$

$$U_{el} = \frac{\lambda}{2}(\varepsilon_{ii}^e)^2 + \mu\varepsilon_{ij}^e\varepsilon_{ij}^e$$

$$\rho = \sqrt{\alpha_{ij}\alpha_{ij}}/b, \alpha_{ij} = \epsilon_{jkl}\beta_{il,k}, \beta_{ij} = \beta s_i m_j$$

The equilibrium state governed by the minimization of the total energy

$$E_T = E_s + E_B, E_B = \int_V U dV$$

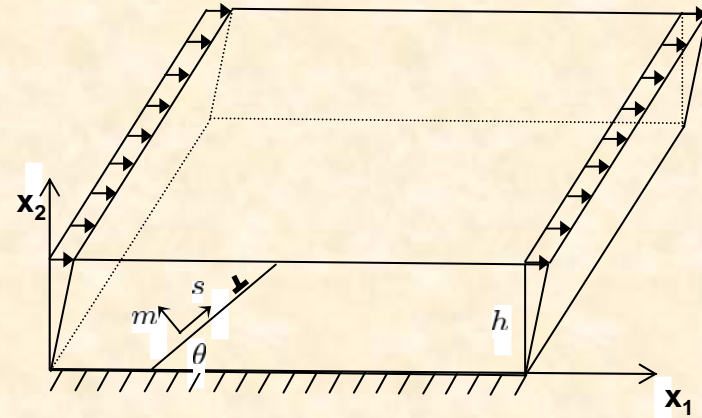
Thin film under plane constrained shear

Prescribed displacements

$$u_1(h) = \gamma h$$

$$u_2(h) = u_1(0) = u_2(0) = 0$$

The total energy in terms of displacements and plastic distortion



$$E_T = \int_V \left[\lambda u_{2,2}^2 / 2 + \mu (u_{1,2} - \beta \cos 2\theta)^2 / 2 + \mu (u_{2,2} - \beta \sin 2\theta / 2)^2 \right. \\ \left. + \mu \beta^2 \sin^2 2\theta / 4 - \mu \eta \ln(1 - |\beta_{,2} \sin \theta| / b \rho_s) \right] dV + \int_{\partial V} \Gamma dA$$

Thin film under shear—Basic equations

Use of approximation

$$-\ln(1 - |\beta_{,2} \sin \theta|/b\rho_s) \approx |\beta_{,2} \sin \theta|/b\rho_s + |\beta_{,2} \sin \theta|^2/2(b\rho_s)^2$$

and the minimization of the total energy lead to

$$(u_{1,2} - \beta \cos 2\theta)_{,2} = 0, [(\lambda + 2\mu)u_{2,2} - \mu\beta \sin 2\theta]_{,2} = 0$$

$$\eta\beta_{,22} \sin^2 \theta / (b\rho_s)^2 - \beta + u_{1,2} \cos 2\theta + u_{2,2} \sin 2\theta = 0$$

and natural boundary conditions (penetrable)

实为
位错
密度

$$\underline{\mu\eta\beta_{,2}(h) \sin^2 \theta / (b\rho_s)^2} = -\text{sgn}(\beta_{,2})\mu\eta|\sin \theta|/b\rho_s - \underline{\partial\Gamma/\partial\beta}$$

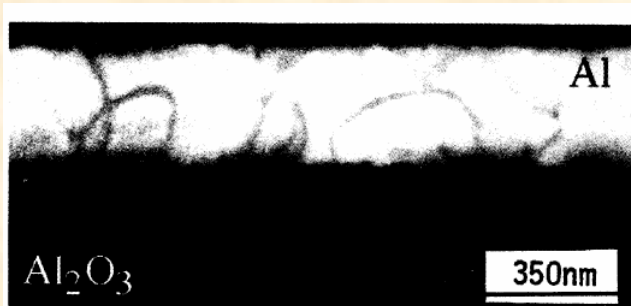
$$\underline{\mu\eta\beta_{,2}(0) \sin^2 \theta / (b\rho_s)^2} = -\text{sgn}(\beta_{,2})\mu\eta|\sin \theta|/b\rho_s + \underline{\partial\Gamma/\partial\beta}$$

But in the conventional **impenetrable** surface/interface (e.g., [Le and Sembring, Arch Appl Mech 2008](#))

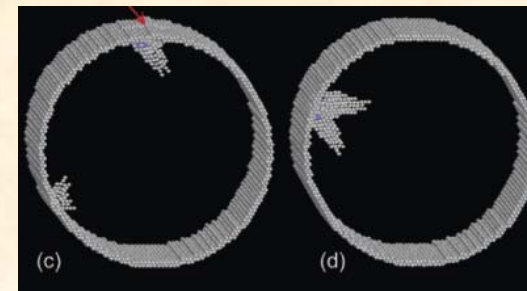
$$\beta(0) = \beta(h) = 0$$

关于表/界面位错可穿透性假设的一点讨论

- 表/界面在一定条件下也可形核发射位错



(Dehm et al J Mater. Sci Tech 2002)



(Rabkin et al Nanoletters 2007)

- 表/界面也可吸收存储位错
- 位错可跨过晶界

Dislocation transmission across a GB (Wang & Sui, APL 94, 021909, 2009)



Dislocation absorption by GB (Serra et al, Acta Mater. 47, 1425-29, 1999)

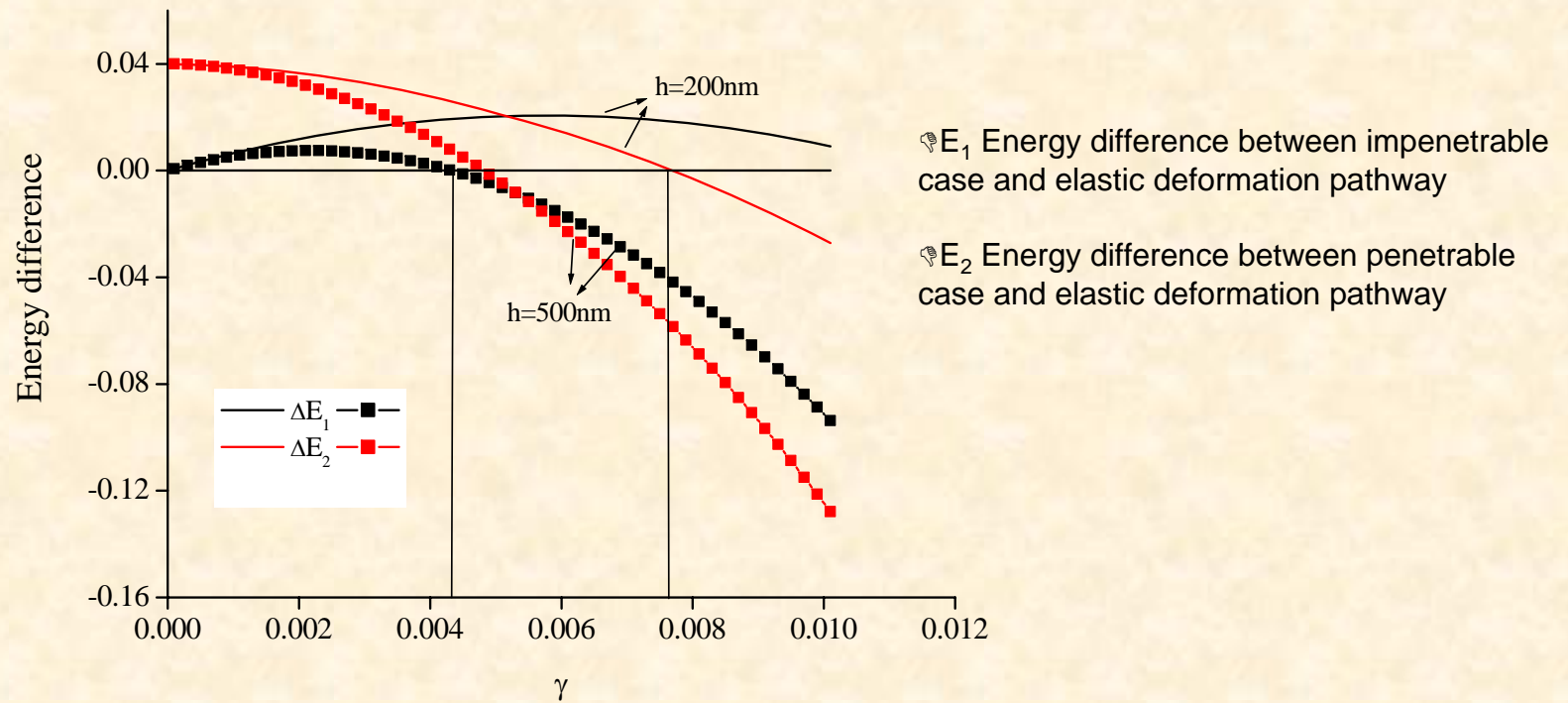
表/界面可能可穿透!

Thin films under plane constrained shear

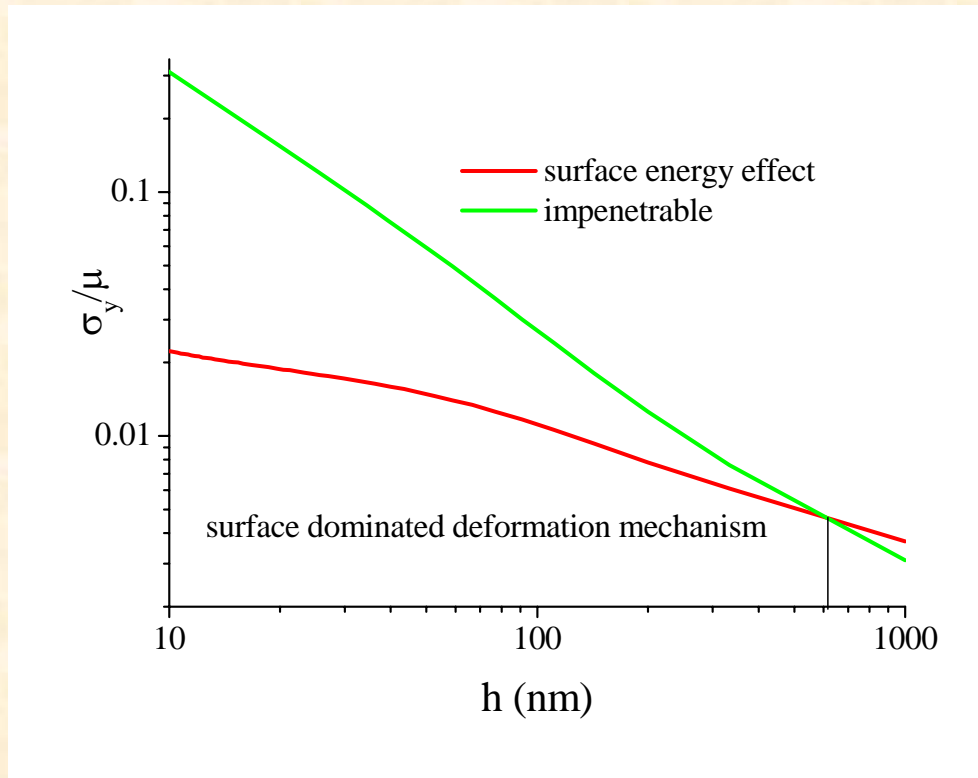
- From Fredriksson & Gudmundson (J Mech Phys Solids 2007)

$$\Gamma = \Gamma_0 |\beta|, \Gamma_0 = \mu b (1 - \ln(b / 2\pi r_0)) / [4\sqrt{3}\pi(1 - \nu)]$$

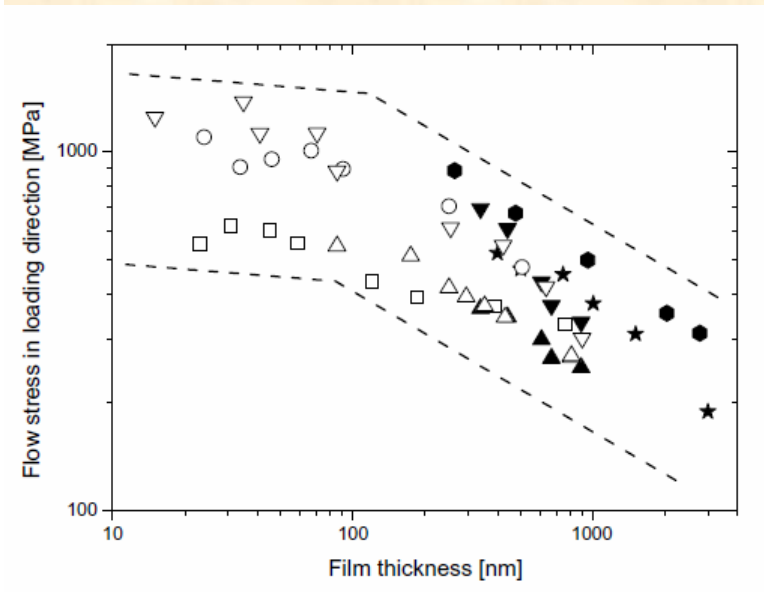
$$\mu = 26.3\text{GPa}, b = 2.5 \times 10^{-10}\text{m}, \eta = 1.138 \times 10^{-3}, \nu = 0.3, \rho_s = 8.8 \times 10^{15}\text{m}^{-2}, \Gamma_0 = 0.4\text{N/m}$$



Thin films under plane constrained shear



Simulation results



Gruber's experiments (Acta Mater 2008)

Surface deformation mechanism dominated in submicrometer-scaled thin films!

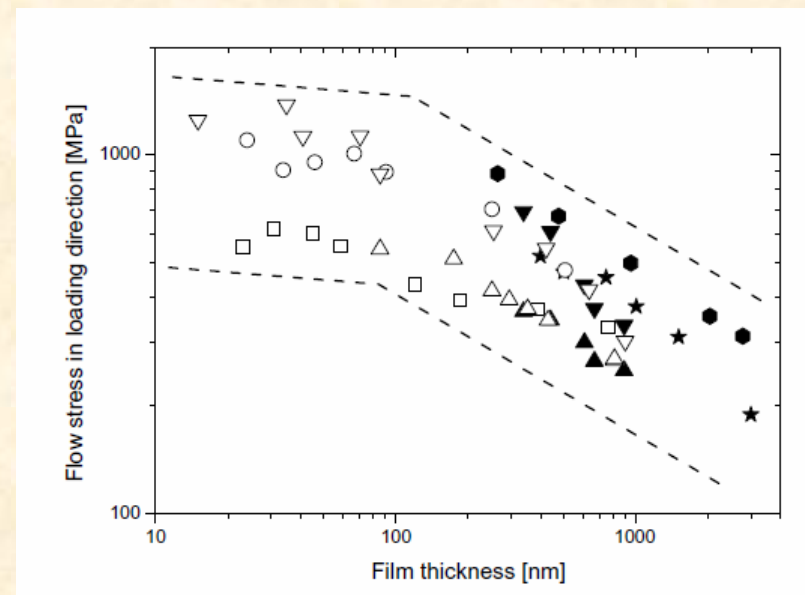
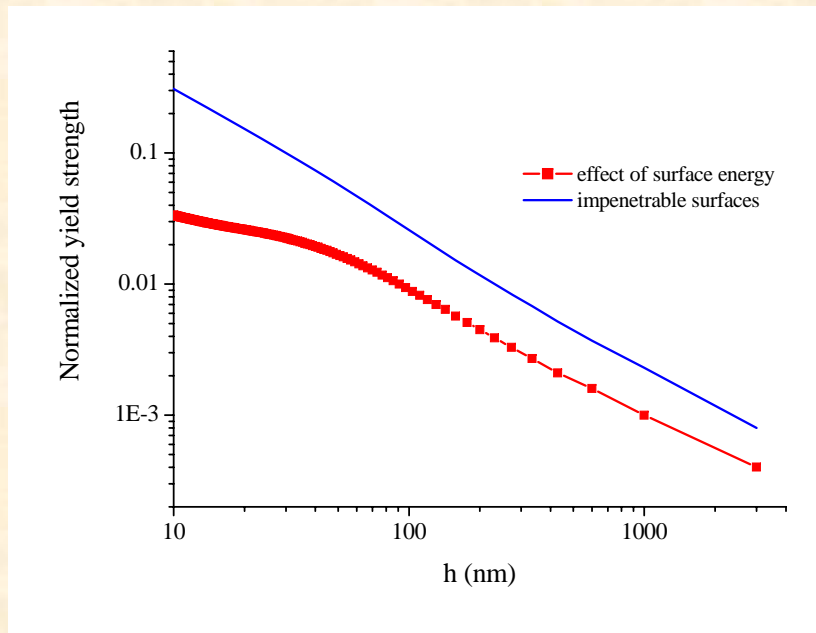
But the dislocation density at the surfaces is constant in the present model!

Thin films under plane constrained shear

- From Gurtin (J Mech Phys Solids 2008)

$$\Gamma = \Gamma_0 \beta^2 / 2,$$

$$\mu = 26.3 \text{ GPa}, b = 2.5 \times 10^{-10} \text{ m}, \eta = 1.138 \times 10^{-3}, \nu = 0.3, \rho_s = 8.8 \times 10^{15} \text{ m}^{-2}, \Gamma_0 = 100 \text{ N/m}$$



Gruber's experiments (Acta Mater 2008)

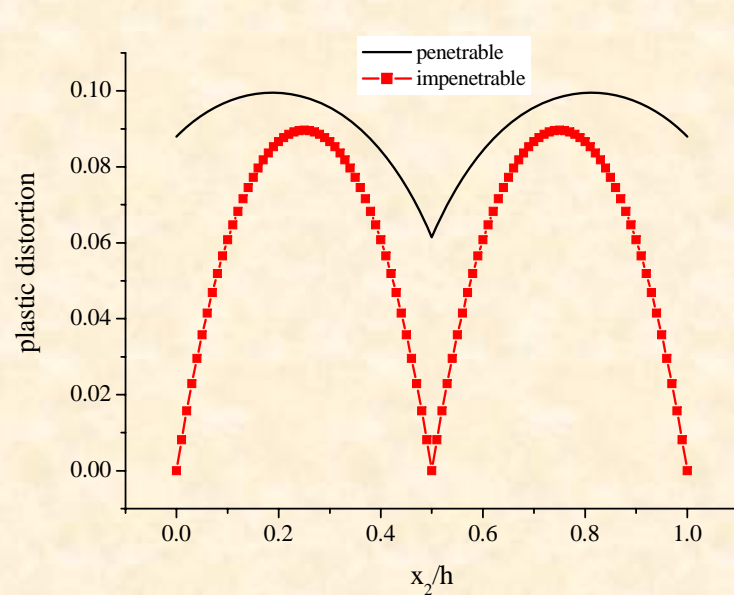
Bicrystal under plane constrained shear

- From Gurtin (J Mech Phys Solids 2008)

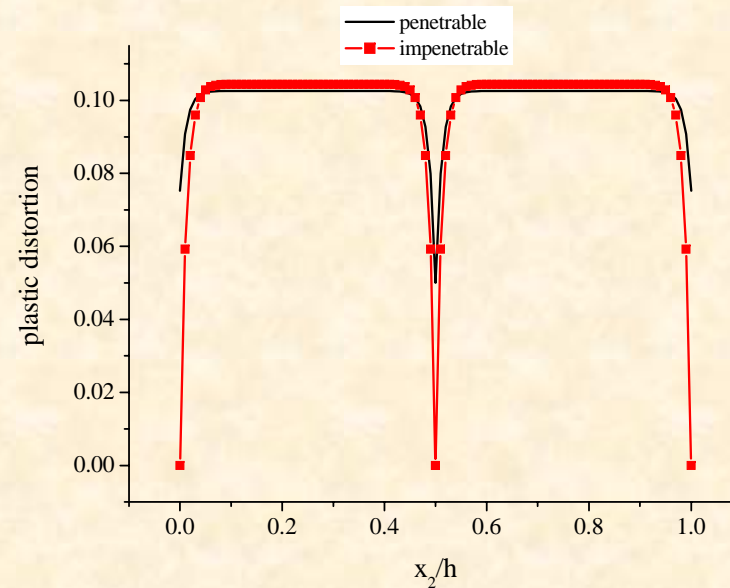
$$\Gamma_{s1} = \Gamma_{10}\beta_1^2 / 2, \Gamma_{s2} = \Gamma_{20}\beta_2^2 / 2, \Gamma_{gb} = \Gamma_{12}(\beta_1^2 \sin^2 \alpha_1 + \beta_2^2 \sin^2 \alpha_2 - 2\beta_1\beta_2 \sin \alpha_1 \sin \alpha_2) / 2$$

$$\mu = 50\text{GPa}, b = 2.5 \times 10^{-10} \text{ m}, \eta = 1.38 \times 10^{-3}, \nu = 0.25, \rho_s = 8.8 \times 10^{15} \text{ m}^{-2}$$

$$\Gamma_{10} = \Gamma_{20} = \Gamma_{12} = 100\text{N/m}, \alpha_1 = \alpha_2 = \pi / 6, \gamma = 0.25$$



$h=2h_1=70 \text{ nm}$



$h=2h_1=1000 \text{ nm}$

Notable effect of surface and interface. Further analysis to be carried out!

Concluding remarks

- Effect of surface and interface plays important roles in size dependent mechanical behavior of nanostructured materials
- Determining the surface parameters experimentally remains challenging
- How the dislocation-surface/interface interaction will affect the plastic behavior in nanocrystalline materials is an interesting problem to be probed
- The effect of surface and interface on the plastic behavior of crystalline materials remains to be further investigated by considering multiple glide systems and rate dependent process.

谢谢大家!
欢迎常到天津大学访问!