微纳结构材料力学行为中的表/界面效应模拟

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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

www.Phys.org

spectrum.ieee.org

www.sandia.gov

www.gizmag.org

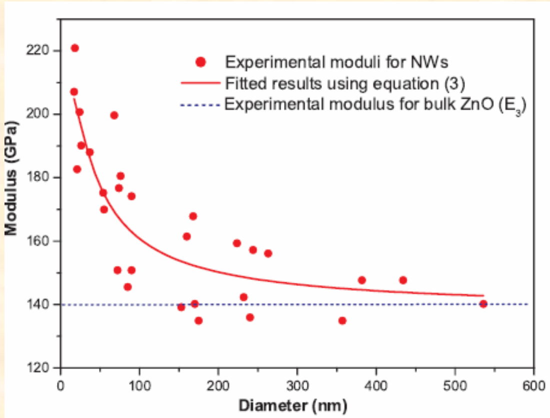
www.voyle.net

www.nsf.gov

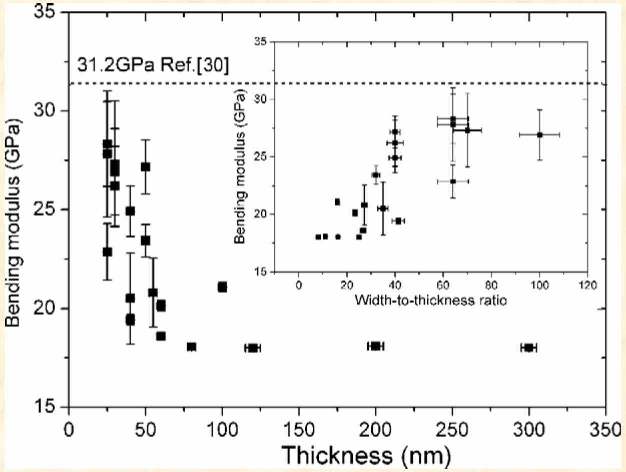
Daoud and Xin Chem Commun. 2005, 2110-2112
Podsiadlo et al. Science, 2007,318,80-83

纳米结构弹性性质的尺寸效应

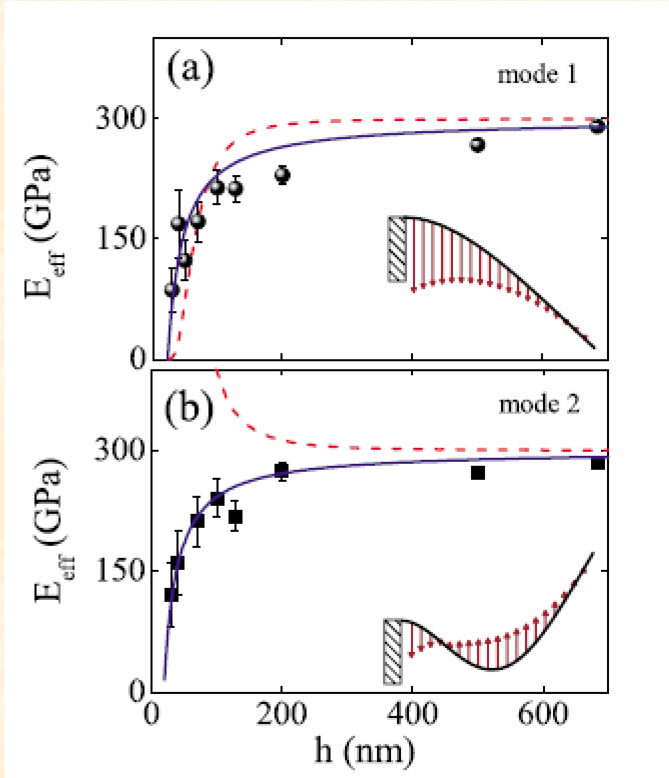
Size dependent moduli of nanostructures



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



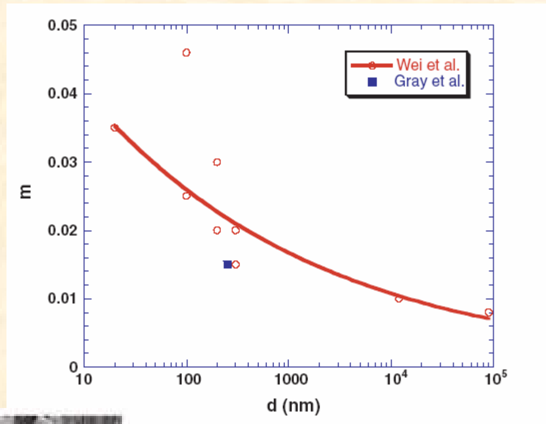
BN Nanosheet [Li et al. Nanotechnology 20, 385707, 2009]

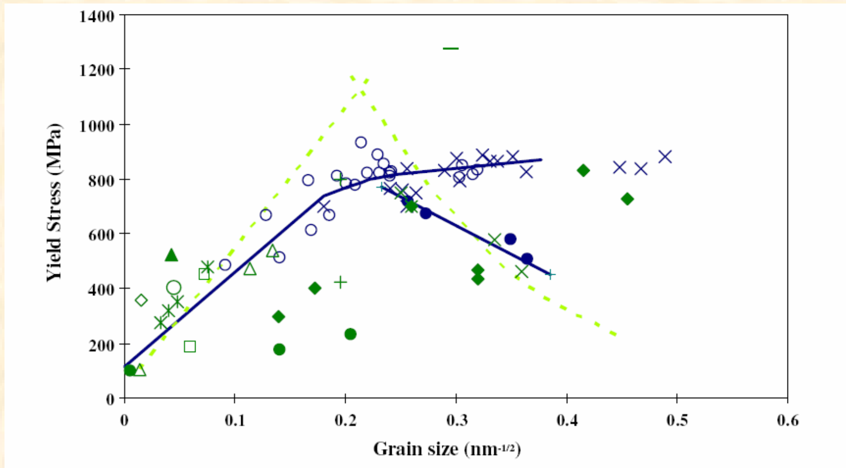


SN cantilever [Gavan et al. APL 94, 233108, 2009]

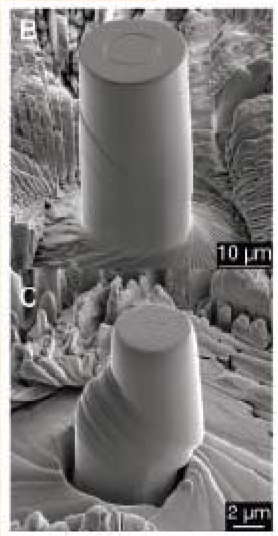
- **Surface/interface effect**
- **Nonlocal effect**
- **Gradient effect**

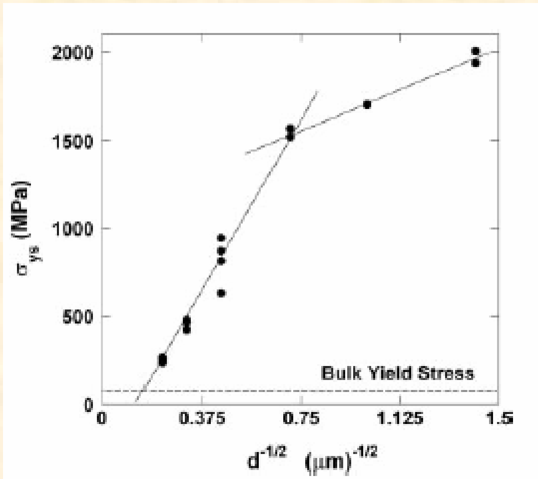
纳米晶体材料塑性行为的尺寸效应





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)

$$\sigma^{s}_{\alpha\beta} = \gamma\delta_{\alpha\beta} + \frac{\partial\gamma}{\partial\varepsilon_{\alpha\beta}} \text{ or } = \sigma^{s0}_{\alpha\beta} + c^{s}_{\alpha\beta\chi\gamma}\varepsilon_{\chi\gamma}$$

Boundary conditions

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

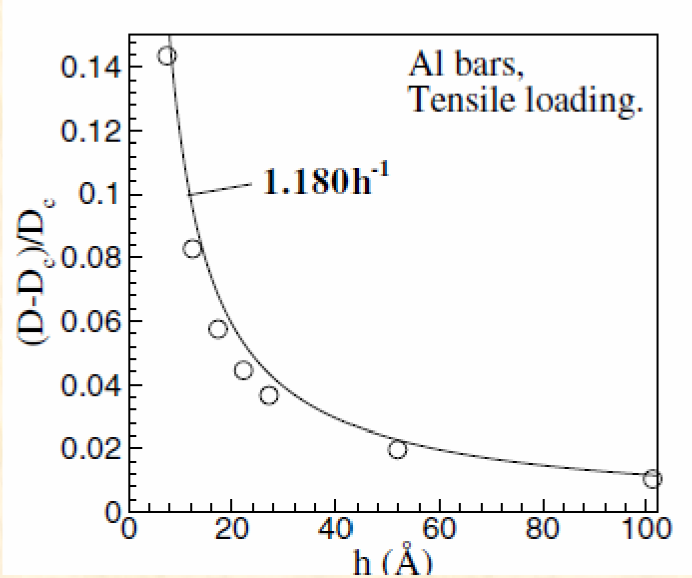
t_α the component of $\sigma_{ij}n_j$ along α direction

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

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

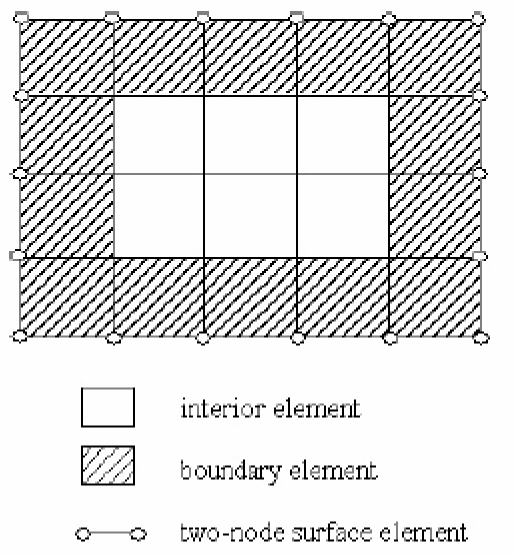
Wang (APL, 2007) and Wang et al (EPL, 2007)

……



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

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



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

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

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

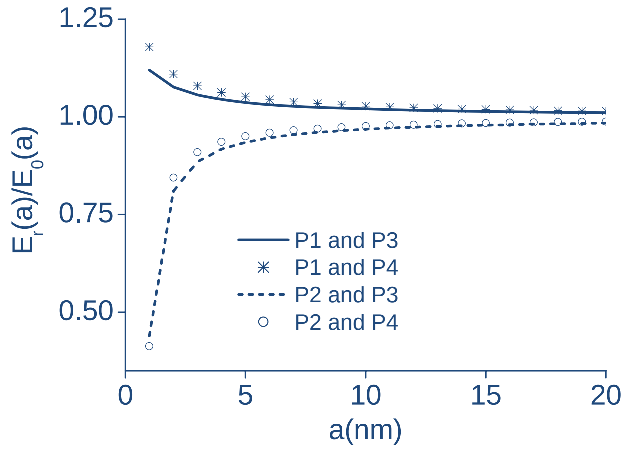
$$[K_e]\{\delta_e\} = \{P_e\} \text{ for elements in the bulk}$$

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

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

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

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



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)

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

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

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

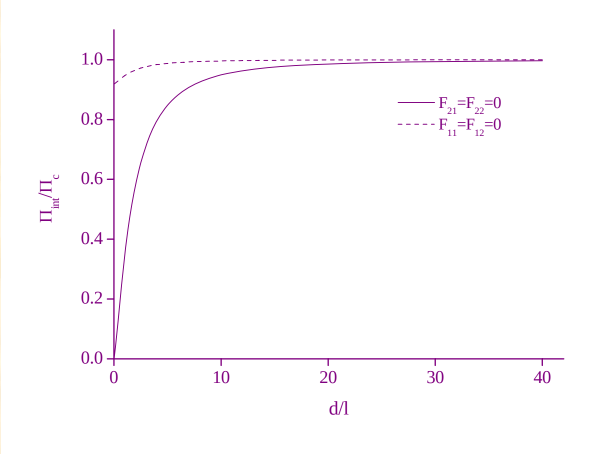
$$u_{13}(x_1, x_3) = \frac{1}{2\pi\mu}\left\{(1-2v)\tan^{-1}\left(\frac{x_3}{x_1}\right) + \frac{1}{2(1-v)}\frac{x_1x_3}{R^2} + (1-2v)\left[\frac{x_3}{2(1-v)} + l\right]g_2\right\},$$

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

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

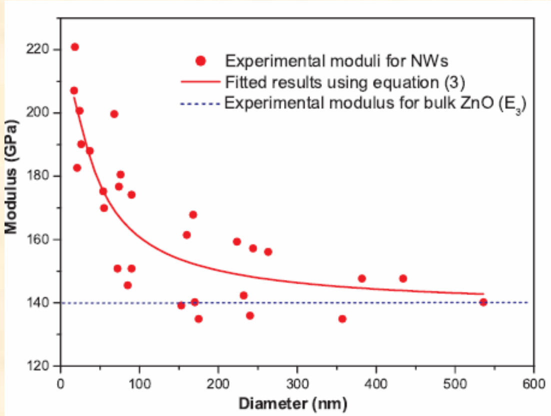
$$R^2 = x_1^2 + x_3^2$$

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

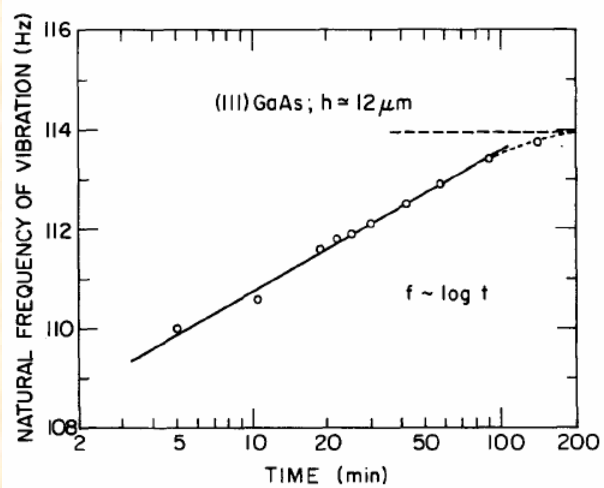


Elastic interaction between steps

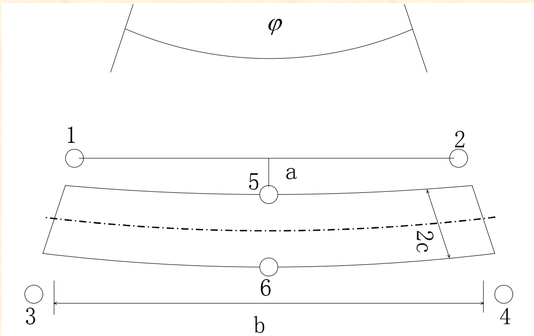
Effect of adsorption on the vibration of a cantilever

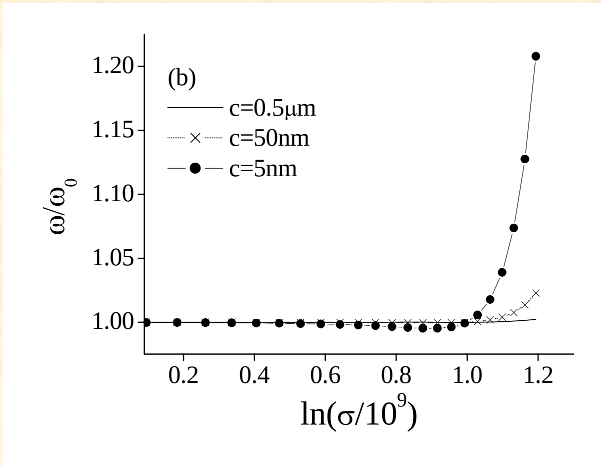


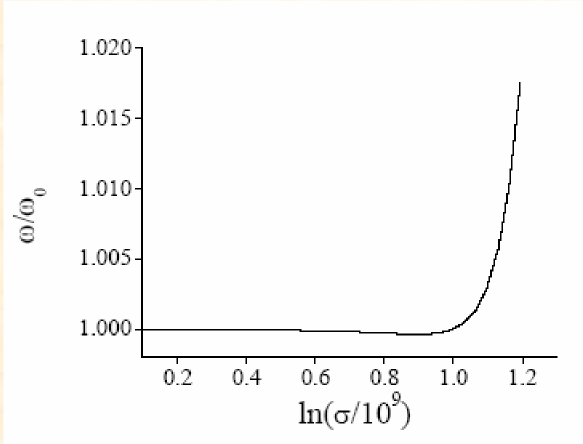
ZnO nanowire[Chen et al. PRL 96, 075505, 2006]



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







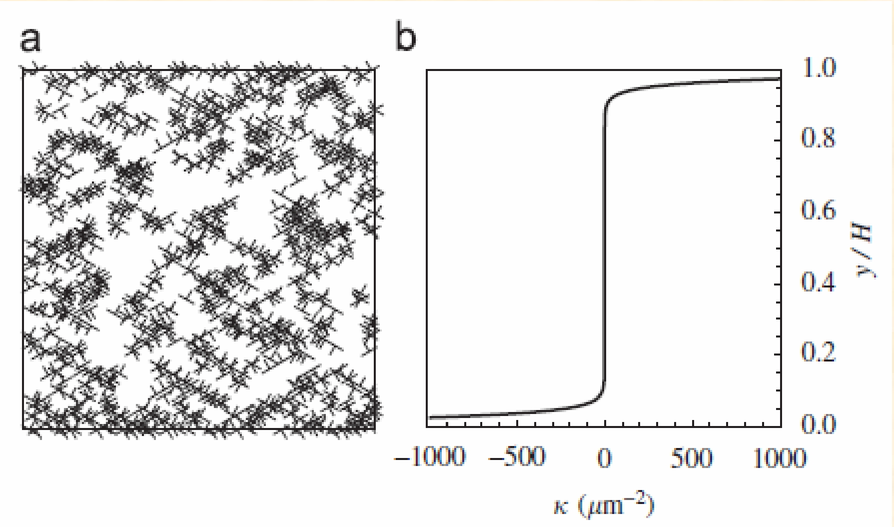
See Huang et al, APL, 89, 043506, 2006

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



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

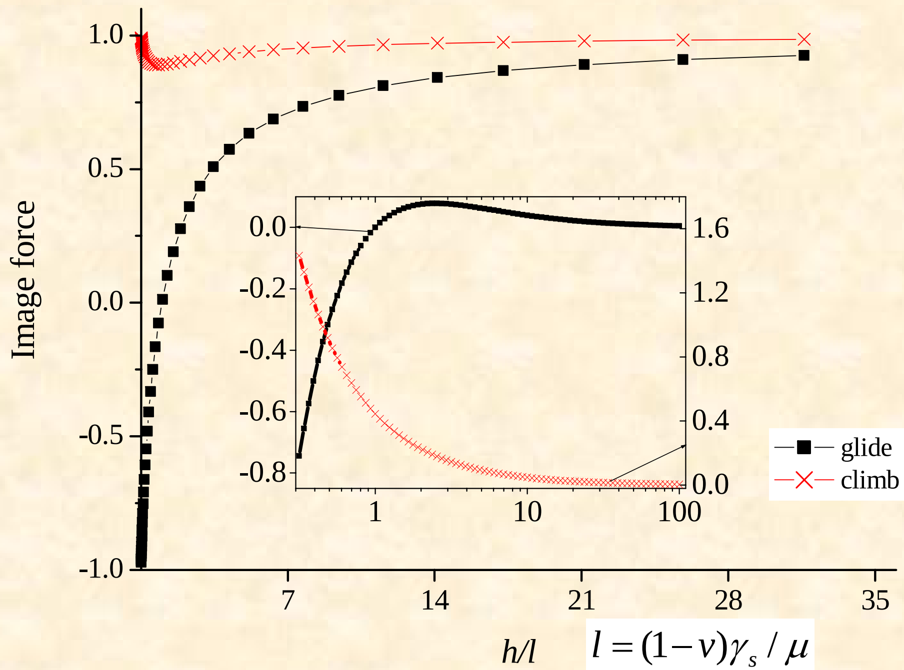
Dislocations are densely distributed near the surface/interface! Influence of surface/interface energy?

Effect of surface energy on the dislocation-surface interaction

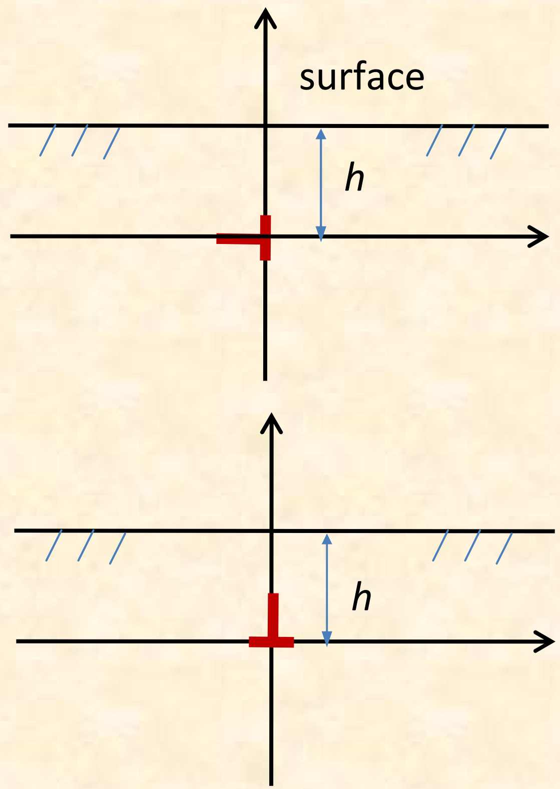
Surface energy: $\int_A \gamma_s \sqrt{1+u_{2,1}^2}\,dx \approx \int_A \gamma_s (1+u_{2,1}^2/2)\,dx$

Boundary conditions

$$\sigma_{22}(x_1,h)=\gamma u_{2,11},\sigma_{21}(x_1,h)=0,$$
$$[u_2(x_1,0)]=b_2H(x_1),[u_1(x_1,h)]=b_1H(x_1),$$



$l=(1-\nu)\gamma_s/\mu$



The image force on the dislocation can be repulsive!

Huang et al, Acta Mech Solida Sinica, 2009

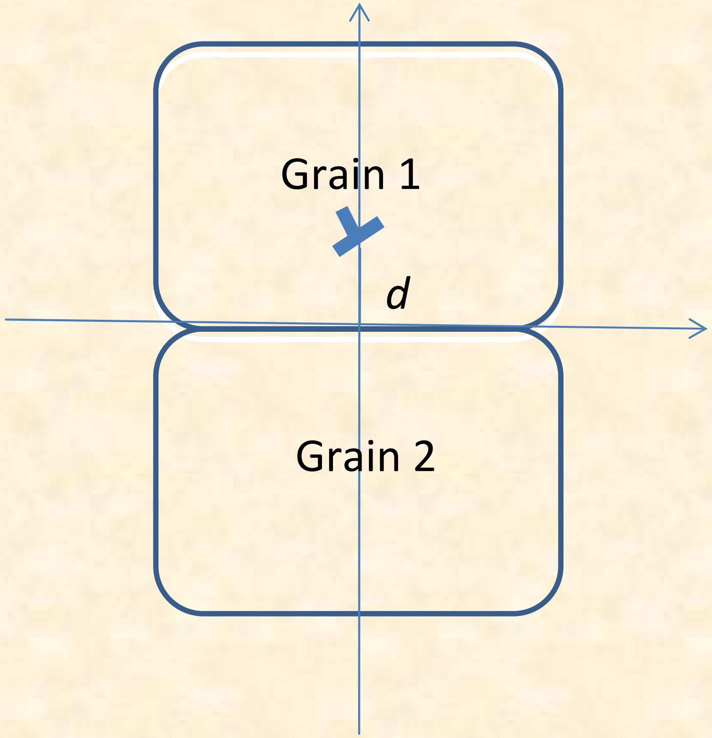
Dislocation-grain boundary interaction by accounting for grain boundary energy

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:

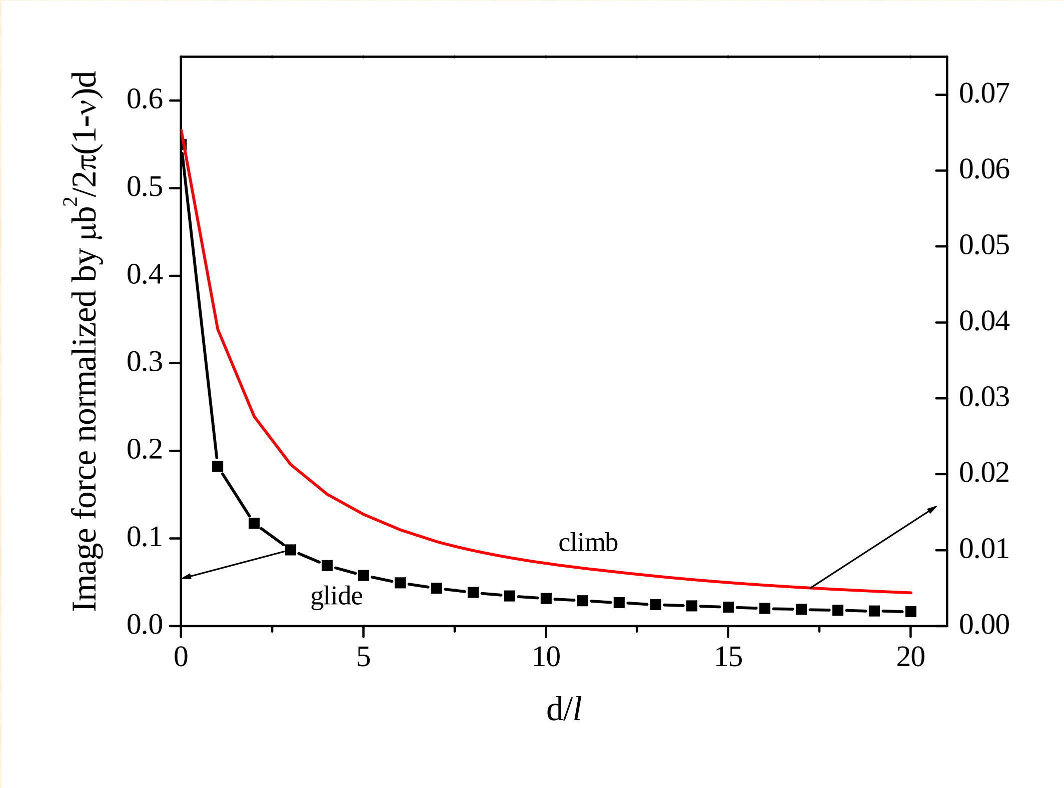
$$U_e = \int_V \sigma_{ij}\varepsilon_{ij}/2dV$$



Boundary conditions:

$$[\sigma_{22}(x_1,0)] = \gamma u_{2,11}, [\sigma_{21}(x_1,0)] = 0, [u_2(x_1,0)] = 0, [u_1(x_1,0)] = 0,$$
$$[\sigma_{22}(x_1,d)] = 0, [\sigma_{21}(x_1,0)] = 0, [u_2(x_1,0)] = b_2H(x_1), [u_1(x_1,0)] = b_1H(x_1),$$

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 Sembirong, 2008)

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

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

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

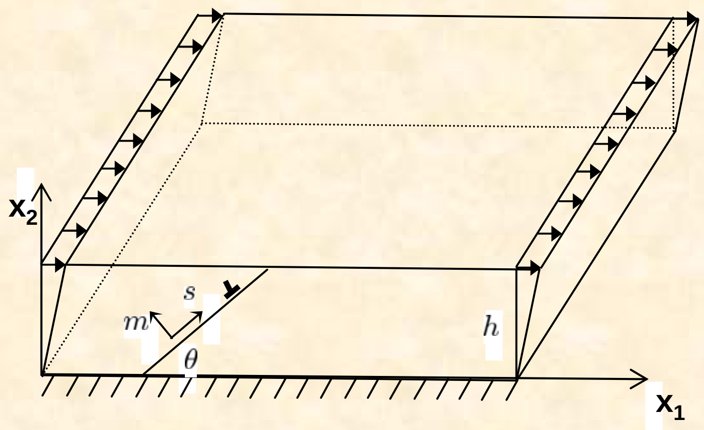
The equilibrium state governed by the mimization of the total energy

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

Thin film under plane constrained shear

Prescribed displacements

$$u_1(h) = \gamma\, h$$
$$u_2(h) = u_1(0) = u_2(h) = 0$$



The total energy in terms of displacements and plastic distortion

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

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

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

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

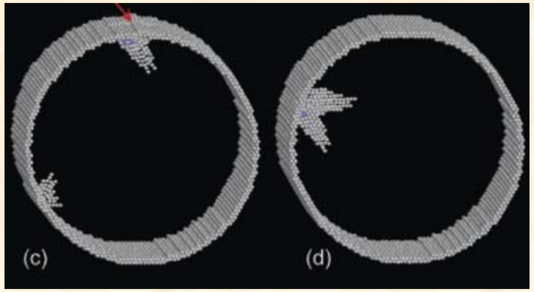
But in the conventional impenetrable surface/interface (e.g., Le and Sembiring, Arch Appl Mech 2008)

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

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)

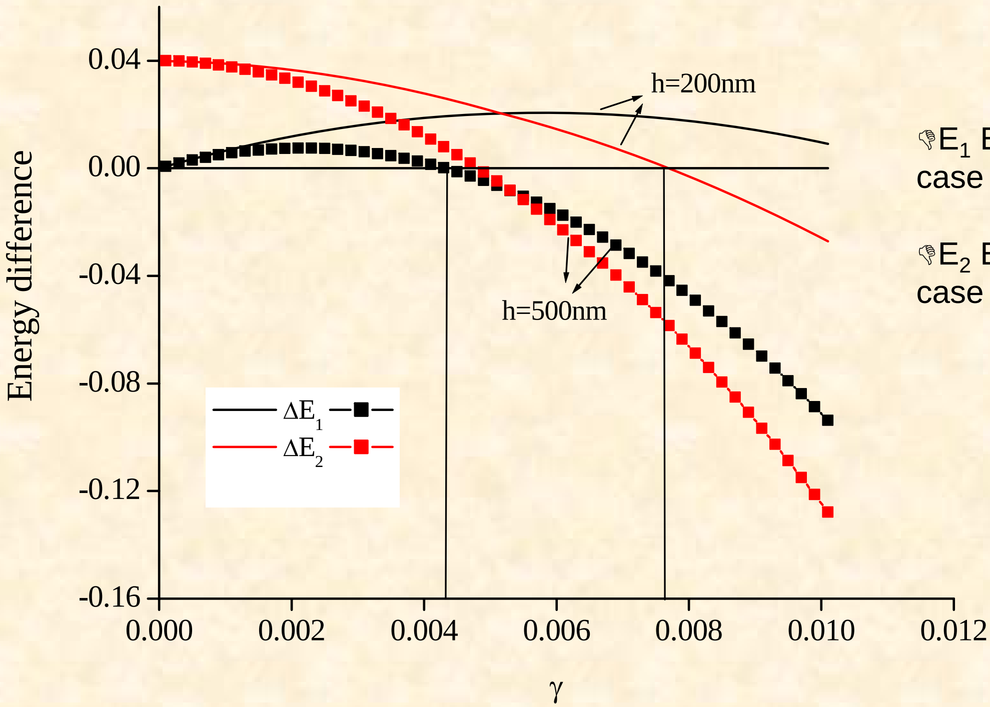
表/界面可能可穿透!

Thin films under plane constrained shear

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

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

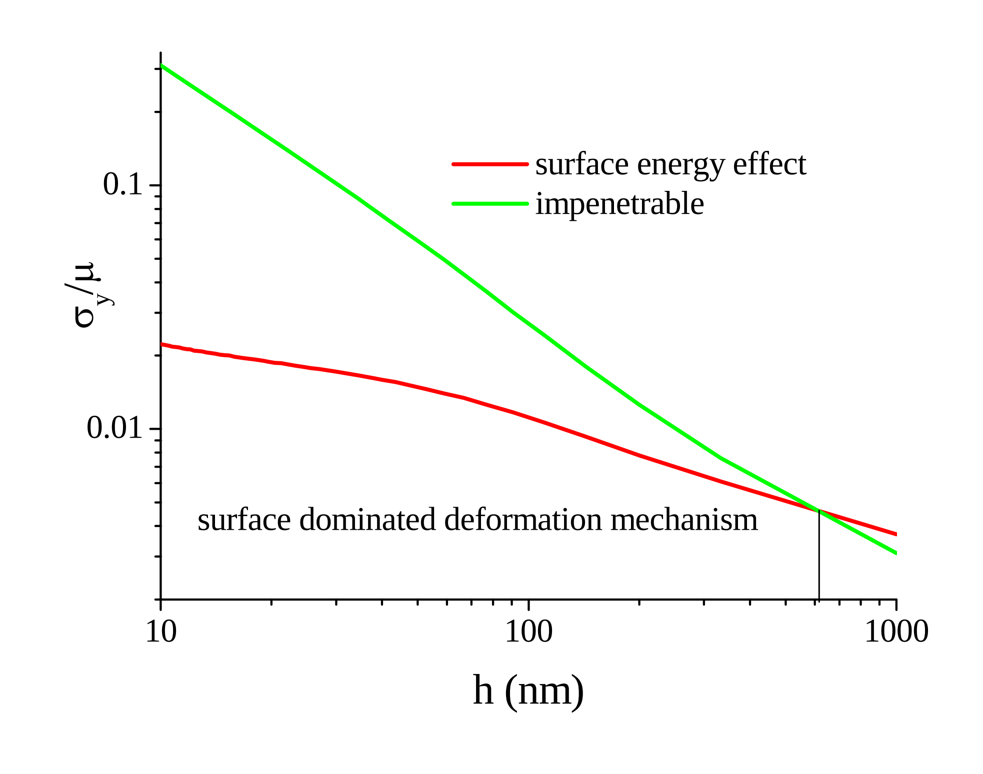
$$\mu = 26.3\text{GPa}, b = 2.5 \times 10^{-10}\text{m}, \eta = 1.138 \times 10^{-3}, \nu = 0.3, \rho_s = 8.8 \times 10^{15}\text{m}^{-2}, \Gamma_0 = 0.4\text{N/m}$$



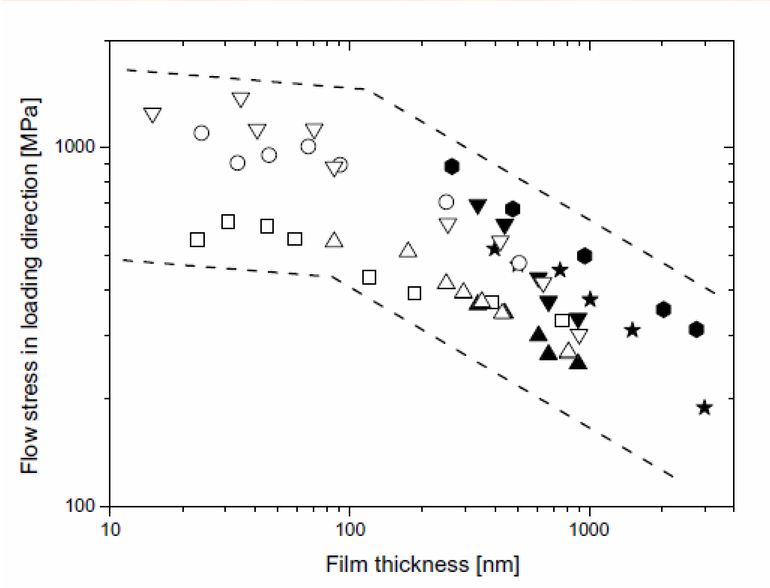
E_1 Energy difference between impenetrable case and elastic deformation pathway

E_2 Energy difference between penetrable case and elastic deformation pathway

Thin films under plane constrained shear



Simulation results



Gruber's experiments (Acta Mater 2008)

Surface deformation mechanism dominated in submicrometer-scaled thin films!

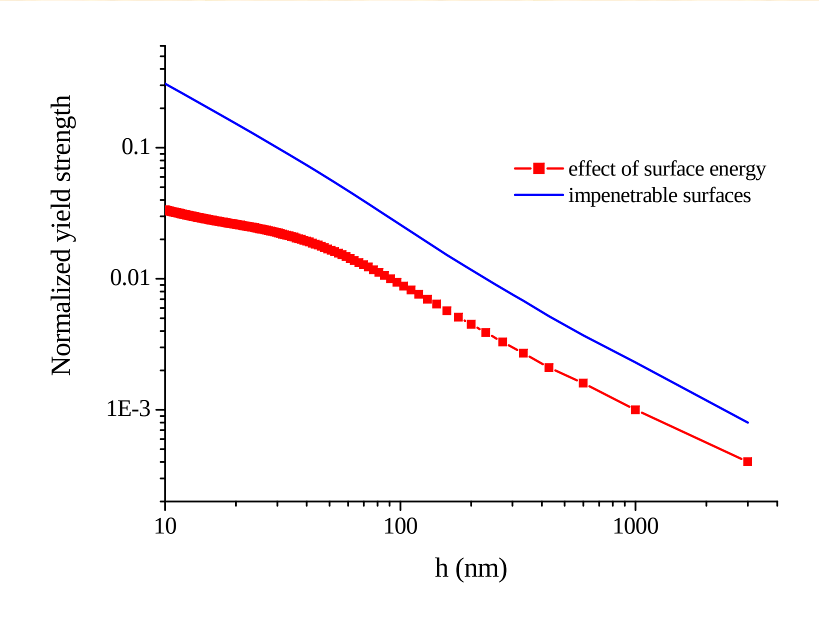
But the dislocation density at the surfaces is constant in the present model!

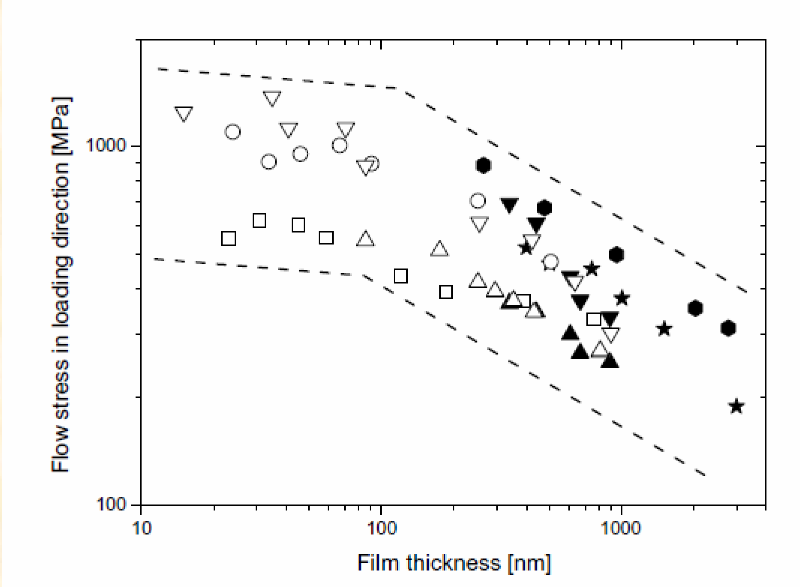
Thin films under plane constrained shear

- From Gurtin (J Mech Phys Solids 2008)

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

$$\mu = 26.3\text{GPa},\ b = 2.5\times10^{-10}\,\text{m}, \eta = 1.138\times10^{-3}, \nu = 0.3, \rho_s = 8.8\times10^{15}\,\text{m}^2, \Gamma_0 = 100\,\text{N/m}$$





Gruber's experiments (Acta Mater 2008)

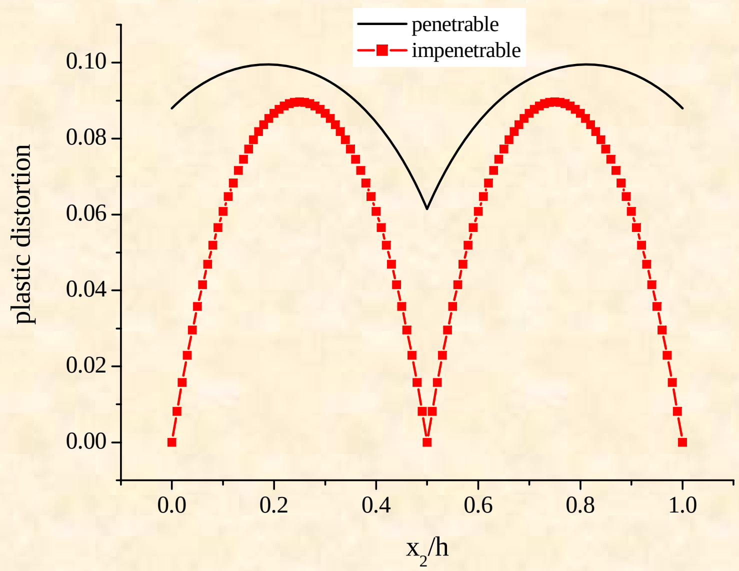
Bicyrstal under plane constrained shear

- From Gurtin (J Mech Phys Solids 2008)

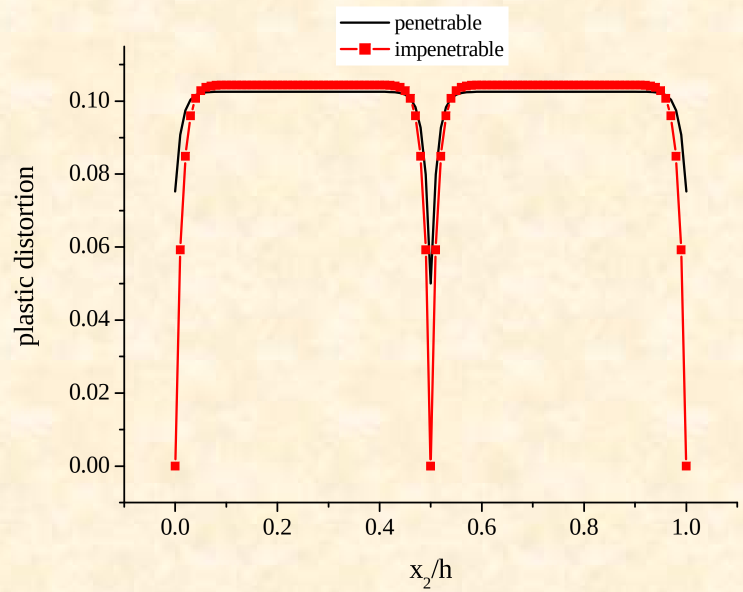
$$\Gamma_{s1} = \Gamma_{10}\beta_1^2/2,\ \Gamma_{s2} = \Gamma_{20}\beta_2^2/2, \Gamma_{gb} = \Gamma_{12}(\beta_1^2\sin^2\alpha_1 + \beta_2^2\sin^2\alpha_2 - 2\beta_1\beta_2\sin\alpha_1\sin\alpha_2)/2$$

$$\mu = 50\text{GPa},\ b = 2.5\times10^{-10}\,\text{m}, \eta = 1.38\times10^{-3}, \nu = 0.25, \rho_s = 8.8\times10^{15}\,\text{m}^2$$

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



h=2h_1=70 nm



h=2h_1=1000 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!