Discrete Dislocation Dynamics and Strain Gradient formulations: a way to model size effects in plasticity

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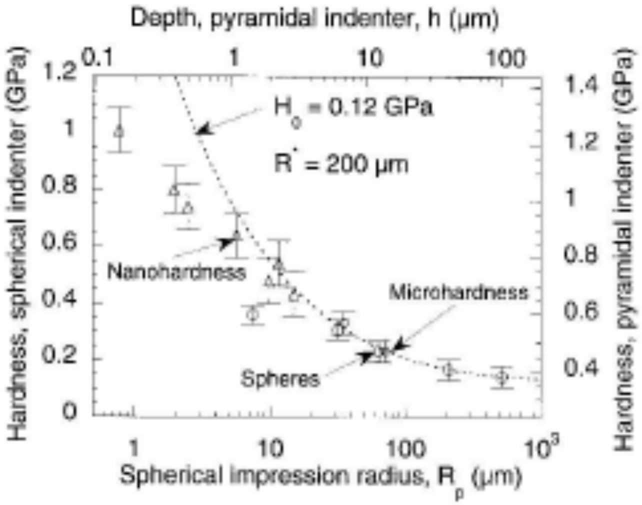
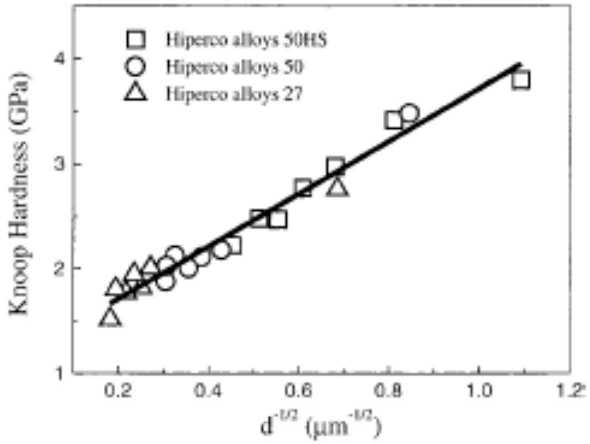
UPMC, Ins. Jean Le Rond D'Alembert 24th June 2010

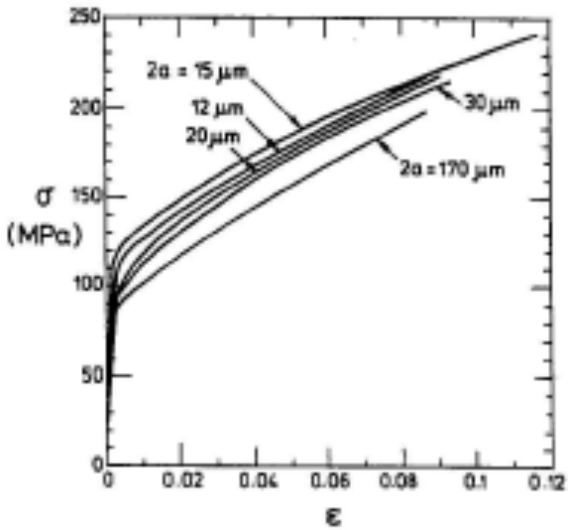
“ Smaller is stronger ???”

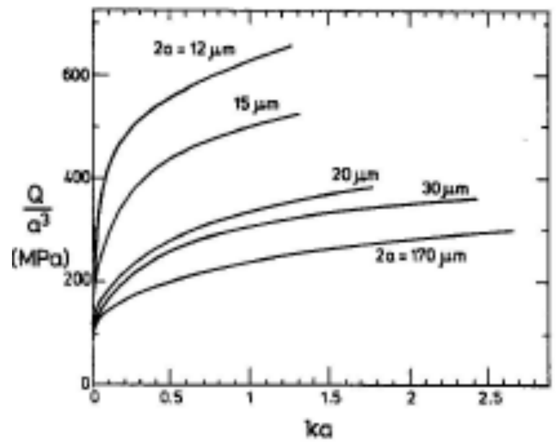
- Theory of conventional plasticity predicts no size effects.
- Experimental evidence indicate that at length scales of a few 10s of microns materials exhibit size effects.
- Size effects due to internal characteristic length scales (e.g., microstructure)
  - Grain size dependence in a polycrystal
  - Reinforcement size dependence in a metal-matrix composite
- Size effects due to the imposed loading conditions
  - Size dependant response of thin films & thin wires
  - Micro- and nano-indentation size effects

Experimentally observed size effects





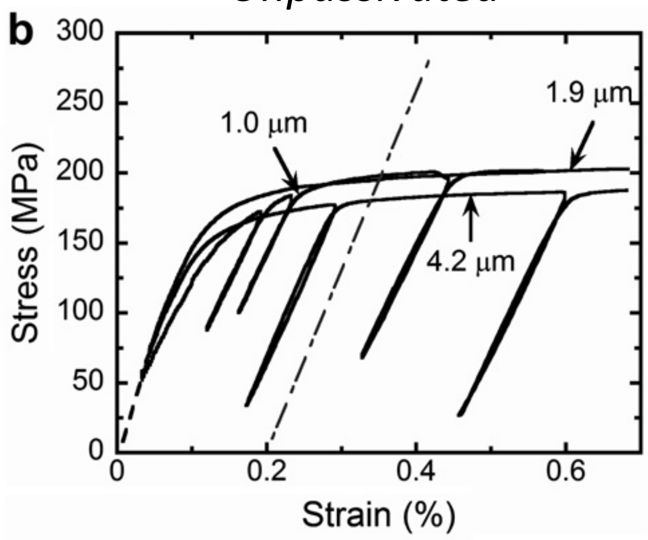




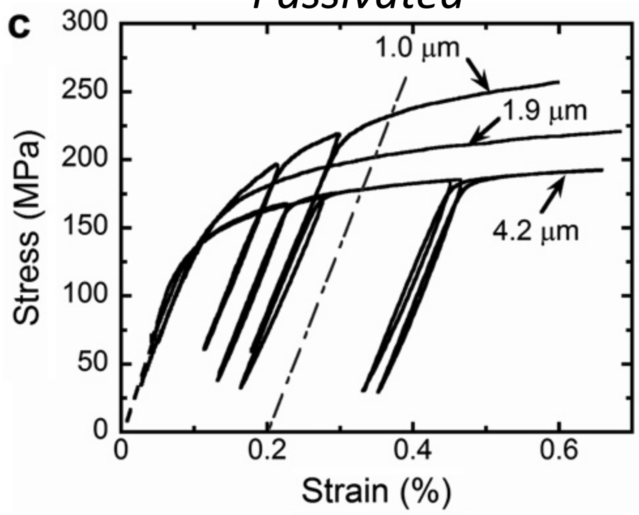
Fleck et al. (1994); Shang et al. (2000); Swadener et al. (2002)

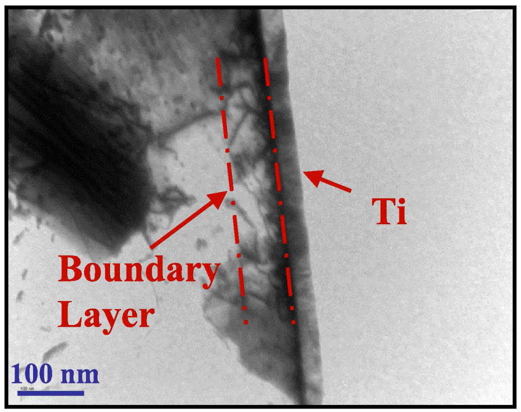
Experimentally observed size effects

Unpassivated

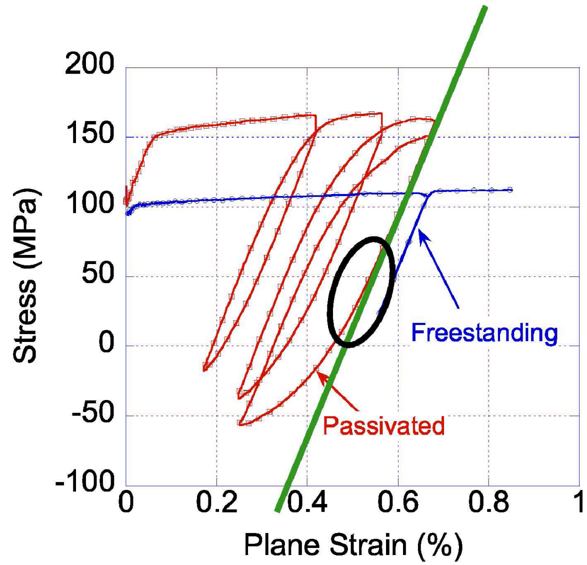


Passivated





TEM micrograph



1 μm Al films

Xiang and Vlassak, (2006)

Why size dependence exists?

- Geometrically necessary dislocations (GNDs) induce strong plastic strain gradients (Ashby, 1970) leading to size effects

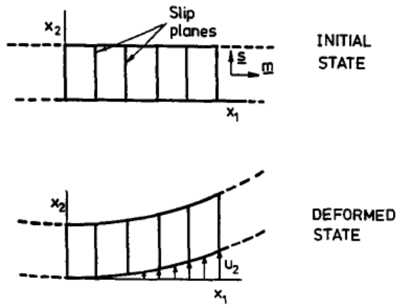


Fig. 3. A beam subjected to non-uniform shear. Plastic slip is assumed to occur on a single slip system with unit normal **m** aligned with the x_1 axis, and slip direction **s** aligned with the x_2 axis.

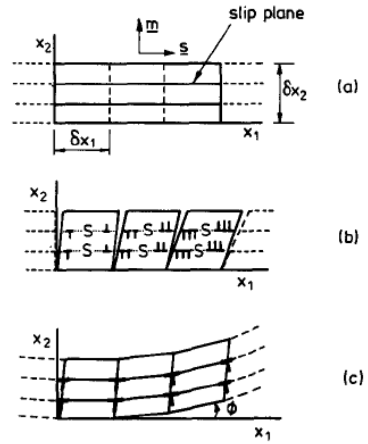
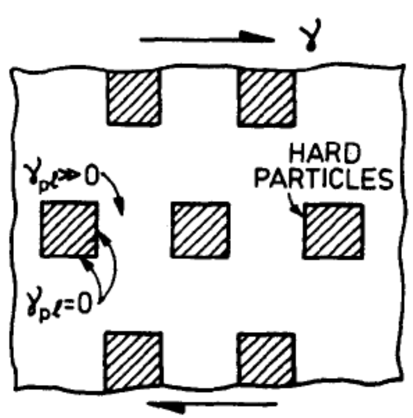
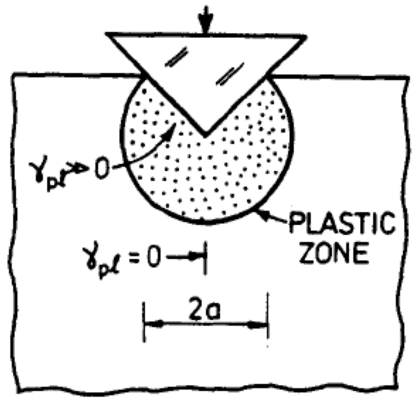


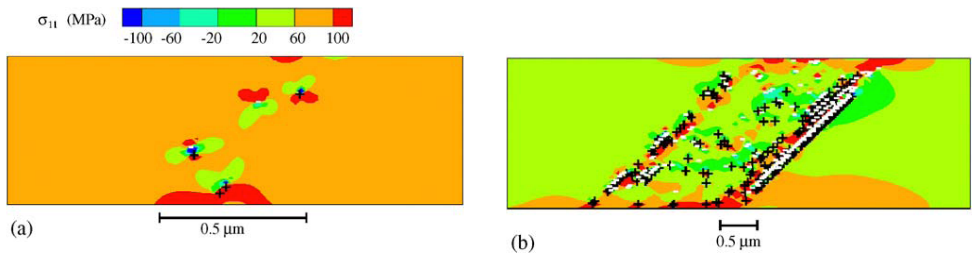
Fig. 4. Sketch showing that a gradient of slip in the x_1 direction causes a density ρ_G of geometrically necessary dislocations to be stored. Plastic slip is assumed to occur on a single slip system with unit normal **m** aligned with the x_2 axis, and slip direction **s** aligned with the x_1 axis.

- Constraints on dislocation glide:
  - Grain boundaries
  - Interfaces (e.g., near reinforcement particles or neutral axis)
  - Boundary layers (thin films, thin wires, etc.)





- Dislocation starvation (Deshpande et al., 2005; Greer and Nix, 2006)



Brief outline – 2 parts

- Discrete and Continuum theories – a brief discussion
  - Discrete Dislocation theories (DD)
  - Strain Gradient Crystal Plasticity theories (SGP)

- Shearing of a thin single crystal with interfaces of finite width
  - What is the effect of the interface compliance on the overall response of the sheared crystal?
  - Do SGP theory reproduces the DD simulations?

- A tensorial Strain Gradient Plasticity theory
  - A three length scale version

- Conical indentation of an isotropic material
  - What is the effect of the different length scale parameters on the indentation response of the material?
  - Is the spherical expansion of a void solution appropriate to reproduce indentation hardness?
  - Do SGP theories reproduce the Nix-Gao experimental trends?

Discrete Dislocation theory (DD)

A brief outline

Mechanics framework - general

- Quasi-static, infinitesimal deformations:

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right),\ \ \sigma_{ij,j} = 0,\ \ \sigma_{ij} = \sigma_{ji}$$

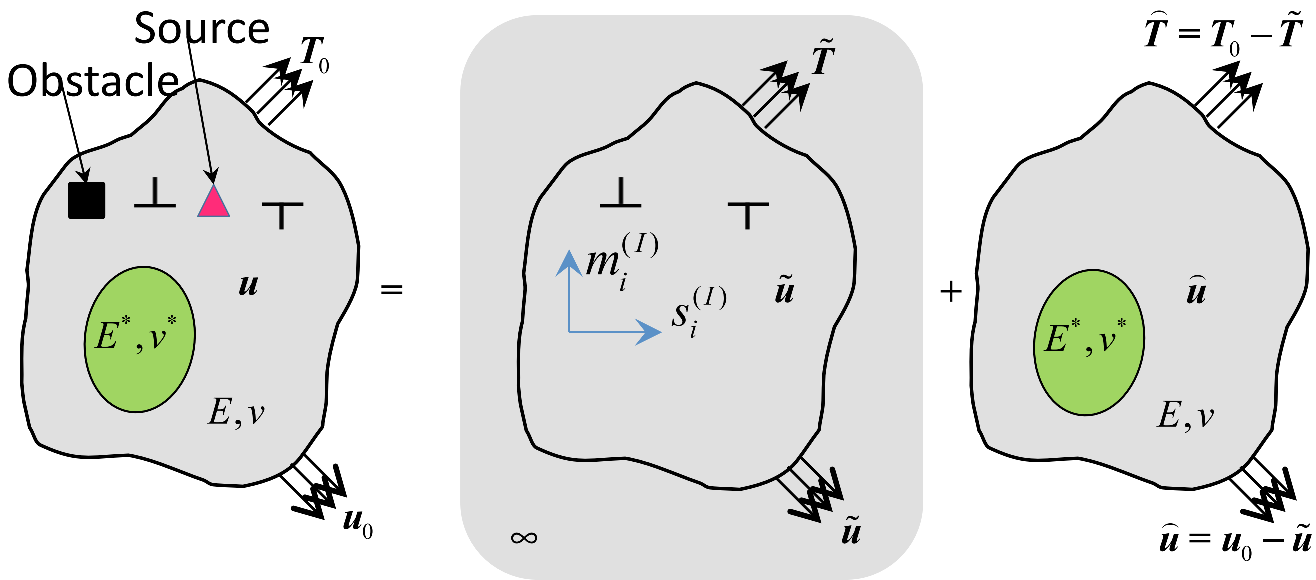
- Isotropic linear elastic material

$$\sigma_{ij} = \frac{E}{1+\nu}\left(\varepsilon_{ij} + \frac{\nu}{1-2\nu}\varepsilon_{kk}\delta_{ij}\right)$$

- Long range interactions come directly from elasticity.

- Sort range interactions obtained via constitutive rules.

Boundary value problems – Plane Strain



- At a given instant in time: $u_i = \tilde{u}_i + \hat{u}_i, \quad \varepsilon_{ij} = \tilde{\varepsilon}_{ij} + \hat{\varepsilon}_{ij}, \quad \sigma_{ij} = \tilde{\sigma}_{ij} + \hat{\sigma}_{ij}$
- (~) fields – sum of the singular equilibrium fields of the individual dislocations

$$\tilde{u}_i = \sum_{J=1}^{N_d} \tilde{u}_i^{(J)}, \quad \tilde{\varepsilon}_{ij} = \sum_{J=1}^{N_d} \tilde{\varepsilon}_{ij}^{(J)}, \quad \tilde{\sigma}_{ij} = \sum_{J=1}^{N_d} \tilde{\sigma}_{ij}^{(J)}, \quad \tilde{\sigma}_{ij,j}^{(J)} = 0$$

- (^) fields – image non-singular fields that correct for the boundary conditions

Van der Giessen and Needleman (1995), Deshpande and coworkers (2001, 2002, 2005, 2008)

DD short range interaction and motion

- Dislocation dipoles with Burgers vector *b* are nucleated at randomly distributed point sources (Frank-Read) when the resolved shear stress takes a value τ_{nuc}.

- The glide component of the Peach-Koehler force, and dislocation motion :

$$f^{(I)} = s_i^{(I)} \left[\hat{\sigma}_{ij} + \sum_{J \neq I} \tilde{\sigma}_{ij}^{(J)} \right] b_j^{(J)}, \qquad \upsilon^{(I)} = f^{(I)} / B_{drag}$$

- Annihilation of two opposite signed dislocations on a slip plane occurs when in a material dependent critical annihilation distance L_e.

- The obstacles to dislocation motion are randomly distributed points on the slip planes. An obstacle releases a pinned dislocation when the Peach-Koehler force on the obstacle exceeds $\tau_{obs}\, b$.

Strain Gradient Crystal Plasticity Theory (SGP)

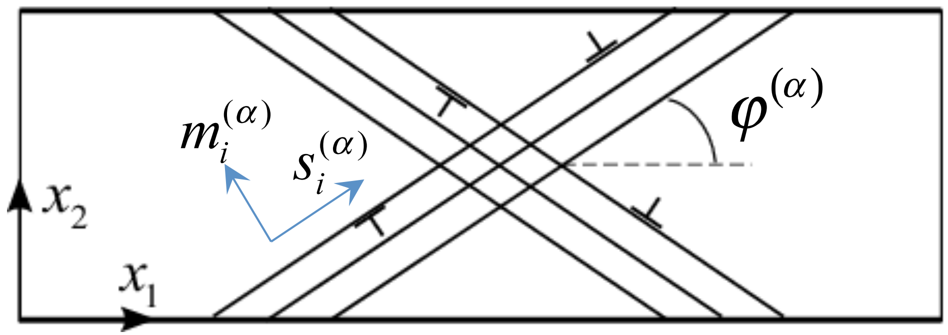
Strain Gradient Crystal Plasticity Theory

- *Kinematics*

$$\dot{\varepsilon}_{ij} = \left(\dot{u}_{i,j}\right)_{symm} = \dot{\varepsilon}^{e}_{ij} + \dot{\varepsilon}^{p}_{ij}, \quad \dot{\varepsilon}^{p}_{ij} = \sum_{\alpha} \dot{\gamma}^{(\alpha)}_{p} \mu^{(\alpha)}_{ij}$$

Schmid orientation tensor:

$$\mu^{(\alpha)}_{ij} = \left(s^{(\alpha)}_{i} m^{(\alpha)}_{j} + m^{(\alpha)}_{j} s^{(\alpha)}_{i}\right)/\,2$$



Slip direction vector

$$s^{(\alpha)}_{i} = \cos\varphi^{(\alpha)} e^{(1)}_{i} + \sin\varphi^{(\alpha)} e^{(2)}_{i}$$

Unit normal of the slip planes

$$m^{(\alpha)}_{i} = -\sin\varphi^{(\alpha)} e^{(1)}_{i} + \cos\varphi^{(\alpha)} e^{(2)}_{i}$$

Gurtin (2002), Borg (2007), Fleck and Willis (2009a)

Strain Gradient Crystal Plasticity Theory

- *Principle of Virtual Work*

Independent variables: $\dot{u}_i, \dot{\gamma}_p^{(\alpha)}, \dot{\gamma}_{p,i}^{(\alpha)}$ → Conjugate variables: $\sigma_{ij}, q^{(\alpha)}, \tau_i^{(\alpha)}$

$$\int_V \left(\sigma_{ij}\delta\dot{\varepsilon}_{ij} + \sum_\alpha \left(q^{(\alpha)} - \sigma_{ij}\mu_{ij}^{(\alpha)}\right)\delta\dot{\gamma}_p^{(\alpha)} + \sum_\alpha \tau_i^{(\alpha)}\delta\dot{\gamma}_{p,i}^{(\alpha)} \right)\mathrm{d}V = \int_S \left(T_i\delta\dot{u}_i + \sum_\alpha t^{(\alpha)}\delta\dot{\gamma}_p^{(\alpha)} \right)\mathrm{d}S$$

Field equations: $\sigma_{ij,j} = 0, \quad q^{(\alpha)} - \tau_{i,i}^{(\alpha)} = \sigma_{ij}\mu_{ij}^{(\alpha)}$

Boundary Tractions: $T_i = \sigma_{ij}n_j, \quad t^{(\alpha)} = \tau_i^{(\alpha)}n_i \quad \text{on} \quad S_t$

Displacement BC: $u = u_0, \quad \dot{\gamma}_p^{(\alpha)} = \dot{\gamma}_p^{(\alpha)0} \quad \text{on} \quad S_u$

Gurtin (2002), Borg (2007), Fleck and Willis (2009a)

Strain Gradient Crystal Plasticity Theory

- *Constitutive equations*

$$U\left(\varepsilon_{ij}^{e},\gamma_{p}^{(\alpha)},\gamma_{p,i}^{(\alpha)}\right)=U_{e}\left(\varepsilon_{ij}^{e}\right)+\sum_{\alpha}U_{p}^{(\alpha)}\left(\gamma_{p}^{(\alpha)},\gamma_{p,i}^{(\alpha)}\right) \Rightarrow \sigma_{ij}=\partial U_{e}/\partial\varepsilon_{ij}^{e}$$

$$q^{(\alpha)}=q^{E(\alpha)}+q^{D(\alpha)},\quad \tau_{i}^{(\alpha)}=\tau_{i}^{E(\alpha)}+\tau_{i}^{D(\alpha)}$$

Energetic terms

$$\gamma_{e}^{(\alpha)}=\left(|\gamma_{p}^{(\alpha)}|^{2}+|L\,\gamma_{p,i}^{(\alpha)}s_{i}^{(\alpha)}|^{2}\right)^{1/2}$$

↑ energetic length scale

defect energy: $U_{p}^{(\alpha)}=\dfrac{G}{2}\left(\gamma_{e}^{(\alpha)}\right)^{2}$

$$q^{E(\alpha)}=\partial U_{p}^{(\alpha)}/\partial\gamma_{p}^{(\alpha)}$$
$$\tau_{i}^{E(\alpha)}=\partial U_{p}^{(\alpha)}/\partial\gamma_{p,i}^{(\alpha)}$$

Dissipative terms

$$\dot{\gamma}_{e}^{(\alpha)}=\left(|\dot{\gamma}_{p}^{(\alpha)}|^{2}+|l\,\dot{\gamma}_{p,i}^{(\alpha)}s_{i}^{(\alpha)}|^{2}\right)^{1/2}$$

↑ dissipative length scale

dissipation potential: $\phi^{(\alpha)}=\dfrac{\sigma_{y}\dot{\gamma}_{0}}{m+1}\left(\dfrac{\dot{\gamma}_{e}^{(\alpha)}}{\dot{\gamma}_{0}}\right)^{m+1}$

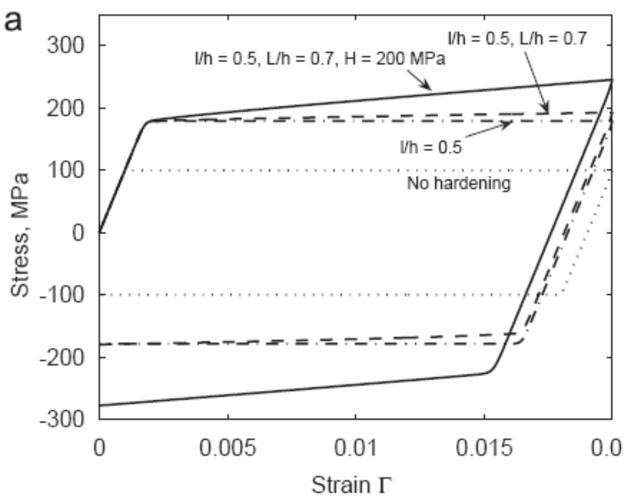
$$q^{D(\alpha)}=\partial\phi^{(\alpha)}/\partial\dot{\gamma}_{p}^{(\alpha)}$$
$$\tau_{i}^{D(\alpha)}=\partial\phi^{(\alpha)}/\partial\dot{\gamma}_{p,i}^{(\alpha)}$$

The sandwiched sheared single crystal problem

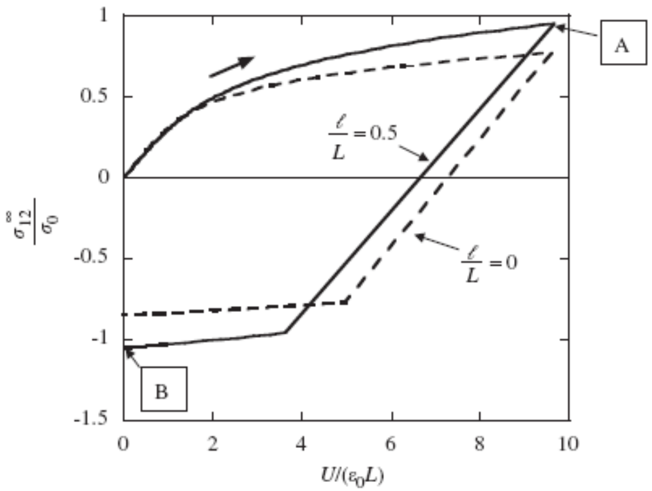
Danas et al., Int. J. of Plasticity, in press

Do sheared single crystals exhibit size effects?

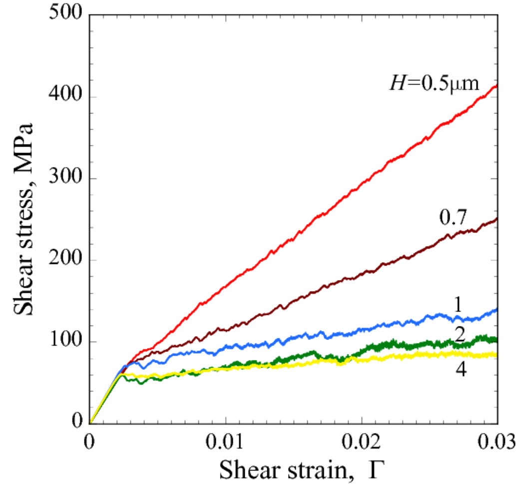
- When a single crystal is under simple shear <u>theoretical results</u> predict strong size effects



Gurtin et al. (2007)



Fleck and Willis (2009a)

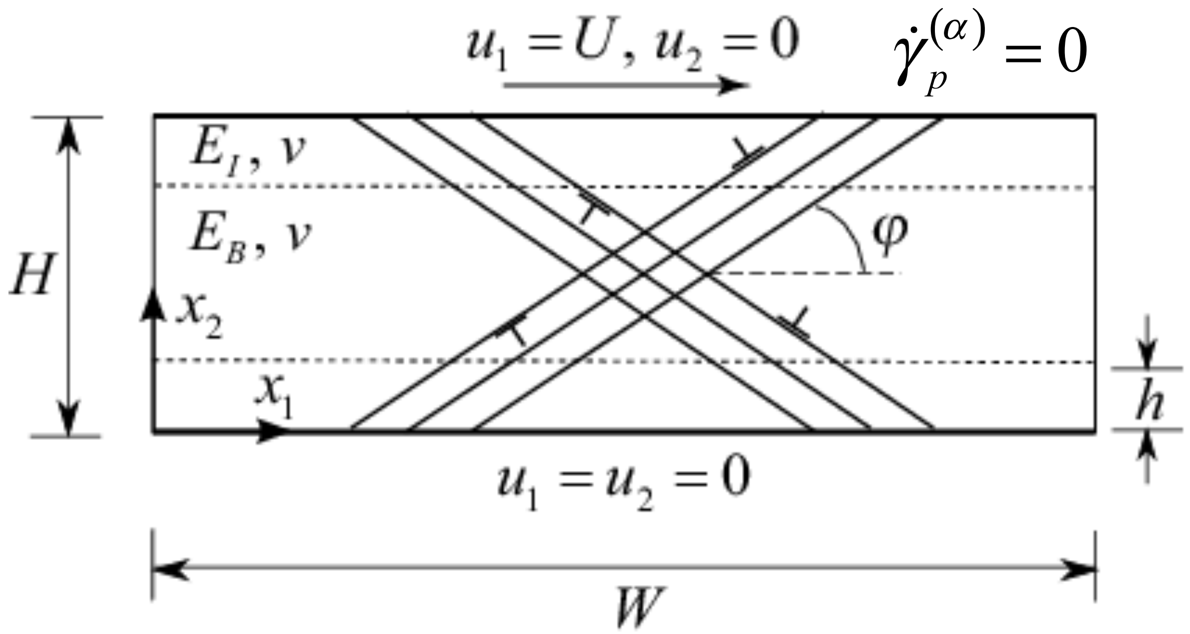


Danas et al. (2010)

- Recent (unpublished) experimental results by Tagarielli and Fleck (2009?) indicate *very small* size effects upon shearing of single aluminium crystals ???

<u>One possible explanation:</u> manufacture of the sandwich specimen (e.g., the joining of two dissimilar solids by diffusion bonding) generates an *interface of finite thickness* with an internal structure that is more amorphous than that of the bulk and consequently more *compliant*.

Model Problem of a prototypical single crystal



Two slip planes

$\alpha = 1, 2, \ \ \varphi^{(\alpha)} = \pm 30^o$

H : height of the crystal

h : height of the interface

E_B : Young's modulus of bulk

E_I : Young's modulus of interface

ν : Poisson ratio

Slip direction vector

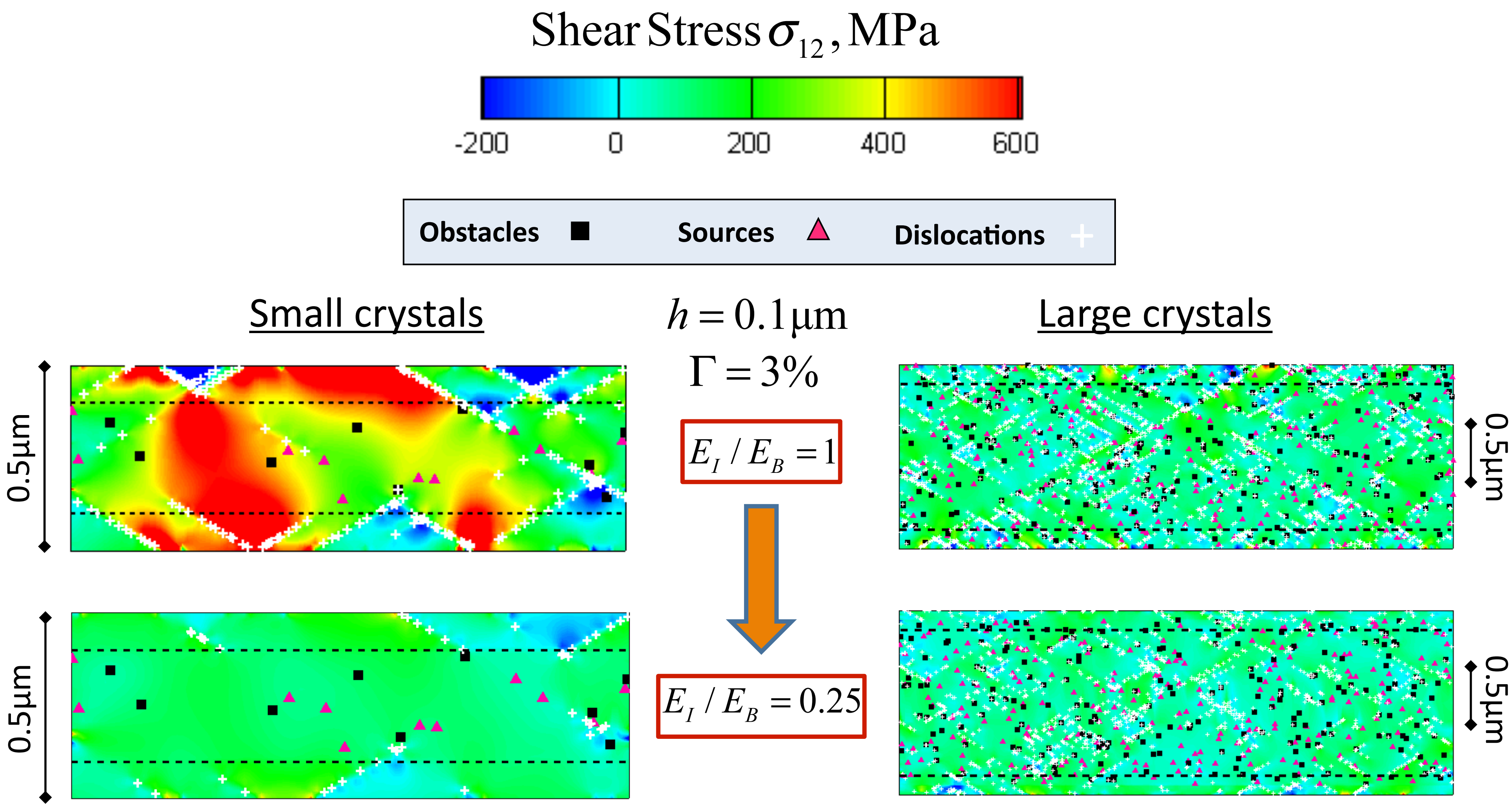
$$s_i^{(\alpha)} = \cos\varphi^{(\alpha)} e_i^{(1)} + \sin\varphi^{(\alpha)} e_i^{(2)}$$

Unit normal of the slip planes

$$m_i^{(\alpha)} = -\sin\varphi^{(\alpha)} e_i^{(1)} + \cos\varphi^{(\alpha)} e_i^{(2)}$$

- Subscripts: B for the bulk crystal & I for the interface
- Plastic response for interface and bulk is the same

Contours of Shear Stress from DD calculations



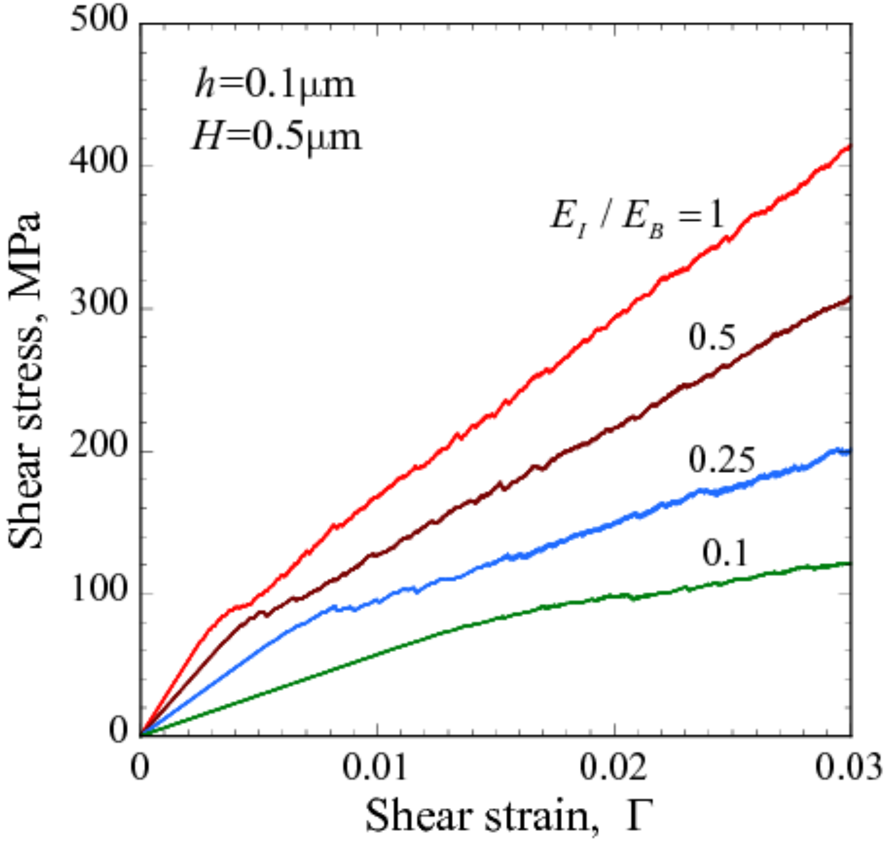
-Higher stresses develop at thinner films due to the back stress generated by dislocation pile-ups inhibiting nucleation throughout the film;

-Additional elastic straining of the film is needed to overcome the back stress.

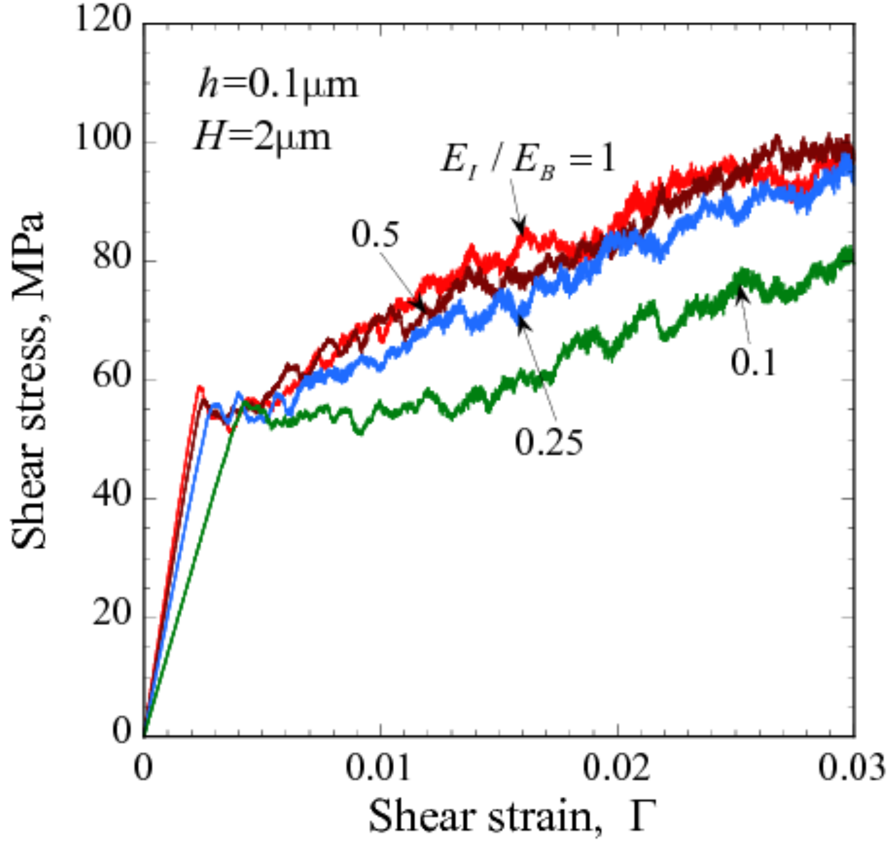
DD Shear Stress – Shear Strain results

Sensitivity analysis of the Young's moduli ratio E_I / E_B

Small crystal



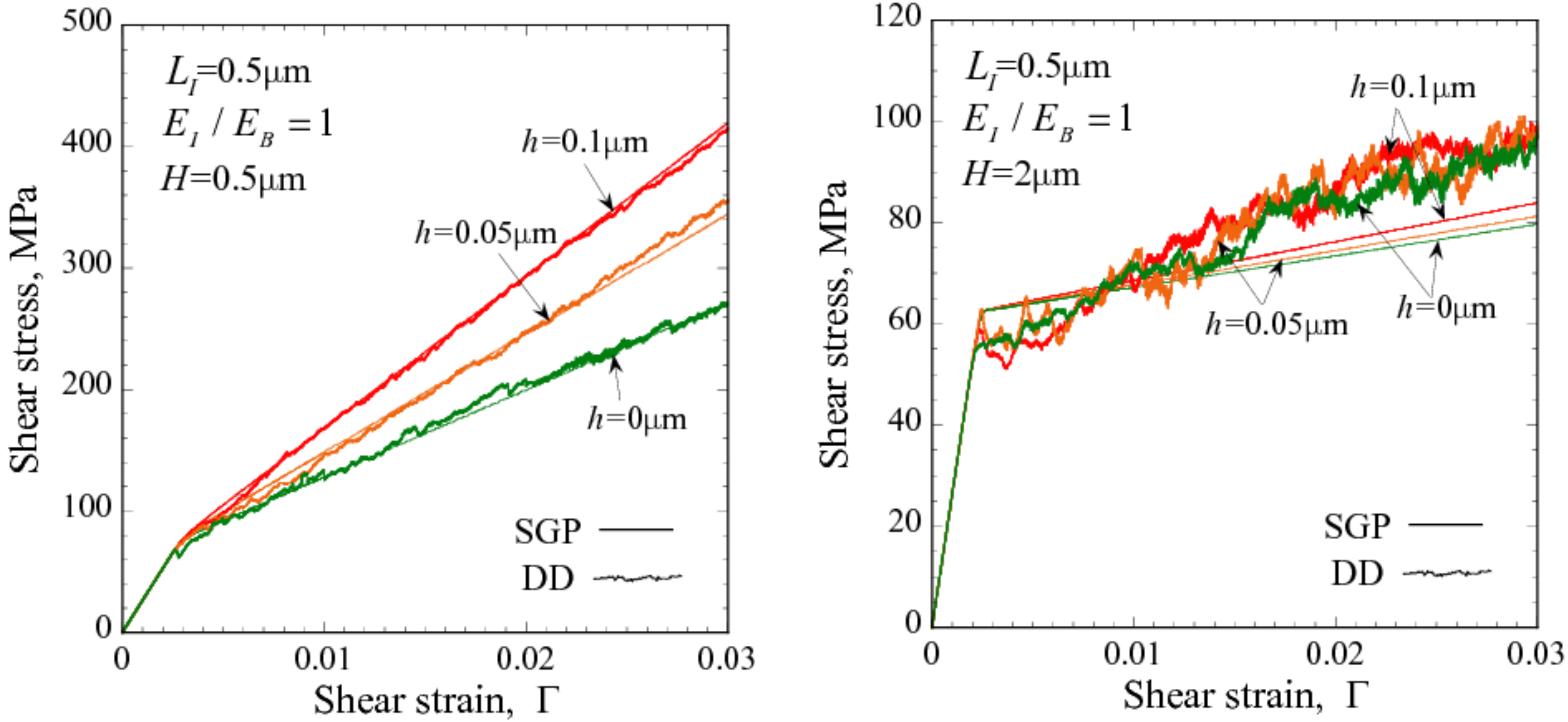
Large crystal



Result: Size effects significantly reduce as interfaces become more compliant!

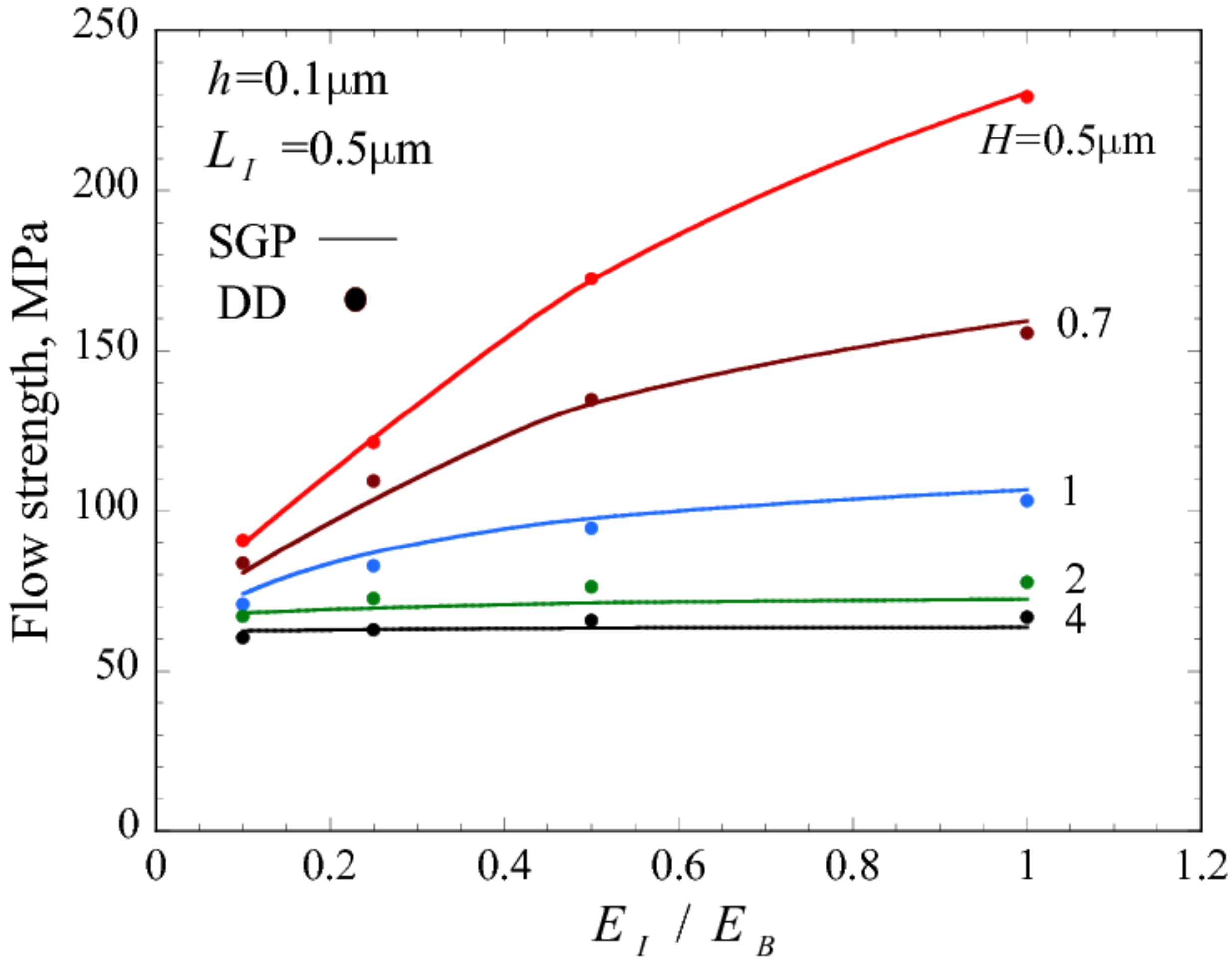
SGP vs. DD results

Sensitivity analysis of the interface height h



In the SGP calculation we use the length scales: $l_I = l_B = L_B = 0.25\mu\text{m},\ L_I = 2\,L_B$

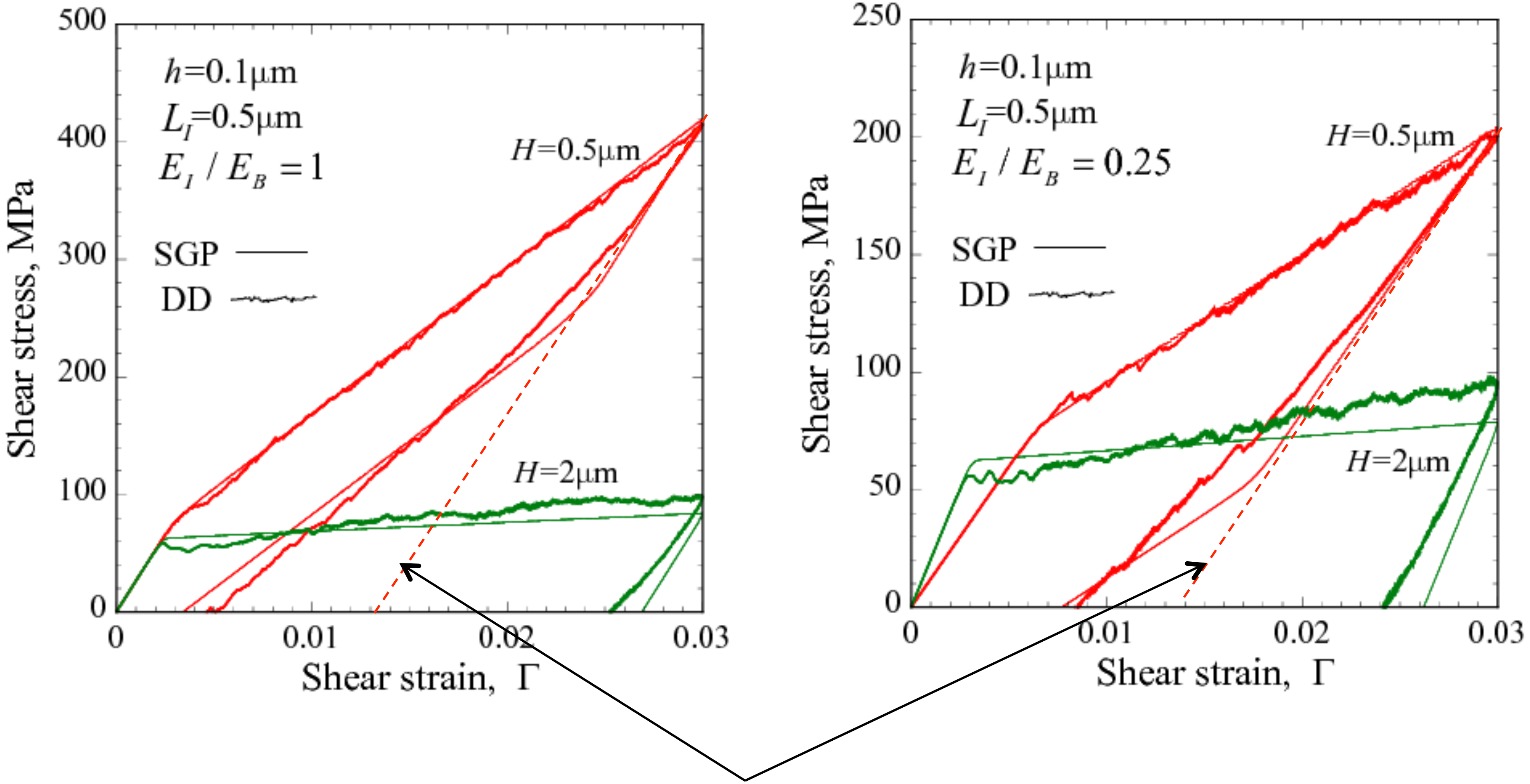
SGP vs. DD flow strength collective results



In the SGP calculation we use the length scales: $l_I = l_B = L_B = 0.25\mu\text{m}, \; L_I = 2L_B$

The flow strength is defined as the average shear stress over the interval $1\% \le \Gamma \le 2\%$

SGP vs. DD unloading curves



If the unloading were linear elastic

Concluding remarks

- When no interfaces are present, dislocation pile-ups form near the boundary surfaces inhibiting further dislocation nucleation. Additional elastic straining is required to overcome this back-stress

- When the interface is more compliant that the bulk crystal this back stress drops significantly. This leads to a significant reduction of both the size effect in the macroscopic shear stress and the Bauschinger effect.

- The SGP is able to reproduce the DD simulations.

<u>2^{nd} Part</u>

The tensorial strain gradient theory

[Gudmundson (2004), Fleck and Willis (2009b)]

⬇

To solve micro-indentation problems

Danas et al., Int. J. of Plasticity, to be submitted

Tensorial Strain Gradient Plasticity Theory

- *Kinematics*

$$\dot{\varepsilon}_{ij} = \left(\dot{u}_{i,j}\right)_{symm} = \dot{\varepsilon}^{e}_{ij} + \dot{\varepsilon}^{p}_{ij}, \quad \dot{\varepsilon}^{p}_{ii} = 0$$

- *Principle of Virtual Work*

Independent variables: $\dot{u}_i, \dot{\varepsilon}^{p}_{ij}, \dot{\varepsilon}^{p}_{ij,k}$ → Conjugate variables: $\sigma_{ij}, q_{ij}, \tau_{ijk}$

$$\int_V \left(\sigma_{ij}\delta\dot{\varepsilon}_{ij} + \left(q_{ij} - \sigma'_{ij}\right)\delta\dot{\varepsilon}^{p}_{ij} + \tau_{ijk}\delta\dot{\varepsilon}^{p}_{ij,k}\right)\mathrm{d}V = \int_S \left(T_i\delta\dot{u}_i + \sum_{\alpha} t_{ij}\delta\dot{\varepsilon}^{p}_{ij}\right)\mathrm{d}S$$

Field equations: $\sigma_{ij,j} = 0, \quad q_{ij} - \tau_{ijk,k} = \sigma'_{ij}$

Boundary Tractions: $T_i = \sigma_{ij}n_j, \quad t_{ij} = \tau_{ijk}n_k \quad \text{on} \quad S_t$

Displacement BC: $u = u_0, \quad \varepsilon^{p}_{ij} = \varepsilon^{p0}_{ij} \quad \text{on} \quad S_u$

Gudmundson (2004), Fleck and Willis (2009b)

Constitutive laws

Elasticity:

$$\sigma_{ij} = \frac{E}{1+v}\left(\varepsilon_{ij}^{e} + \frac{v}{1-2v}\varepsilon_{kk}^{e}\delta_{ij}\right)$$

Effective plastic strain-rate:

Fleck and Hutchinson (1997)

$$\dot{\varepsilon}_{ij,k}^{p} = \rho_{ijk} = \rho_{jik} \quad \Rightarrow \quad \dot{E}_p = \sqrt{\frac{2}{3}\left(\dot{\varepsilon}_{ij}^{p}\dot{\varepsilon}_{ij}^{p} + l_1^2 I_1 + 4 l_2^2 I_2 + \frac{8}{3} l_3^2 I_3\right)}$$

$$I_1 = \rho_{ijk}^{S}\rho_{ijk}^{S} - \frac{4}{15}\rho_{kii}\rho_{kjj}, \quad I_2 = \frac{1}{3}\left(\chi_{ij}\chi_{ij} + \chi_{ij}\chi_{ji}\right), \quad I_3 = \frac{3}{5}\left(\chi_{ij}\chi_{ij} - \chi_{ij}\chi_{ji}\right), \; \chi_{ij} = e_{iqr}\rho_{jrq}$$

Dissipation potential and stress measures:

$$\phi\left(\dot{\varepsilon}_{ij}^{p}, \dot{\varepsilon}_{ij,k}^{p}\right) = \frac{\sigma_y\left(E_p\right)\dot{\varepsilon}_0}{m+1}\left(\frac{\dot{E}_p}{\dot{\varepsilon}_0}\right)^{m+1} \quad \Rightarrow \quad \begin{aligned} q_{ij} &= \partial\phi / \partial\dot{\varepsilon}_{ij}^{p} \\ \tau_{ijk} &= \partial\phi / \partial\dot{\varepsilon}_{ij,k}^{p} \end{aligned}$$

Hardening law:

$$\sigma_y\left(E_p\right) = \sigma_0\left(1 + E_p / \varepsilon_0\right)^N, \quad \varepsilon_0 = \sigma_0 / E, \quad E_p = \int_0^t \dot{E}_p \, \mathrm{d}t$$

Choices for the length scale parameters

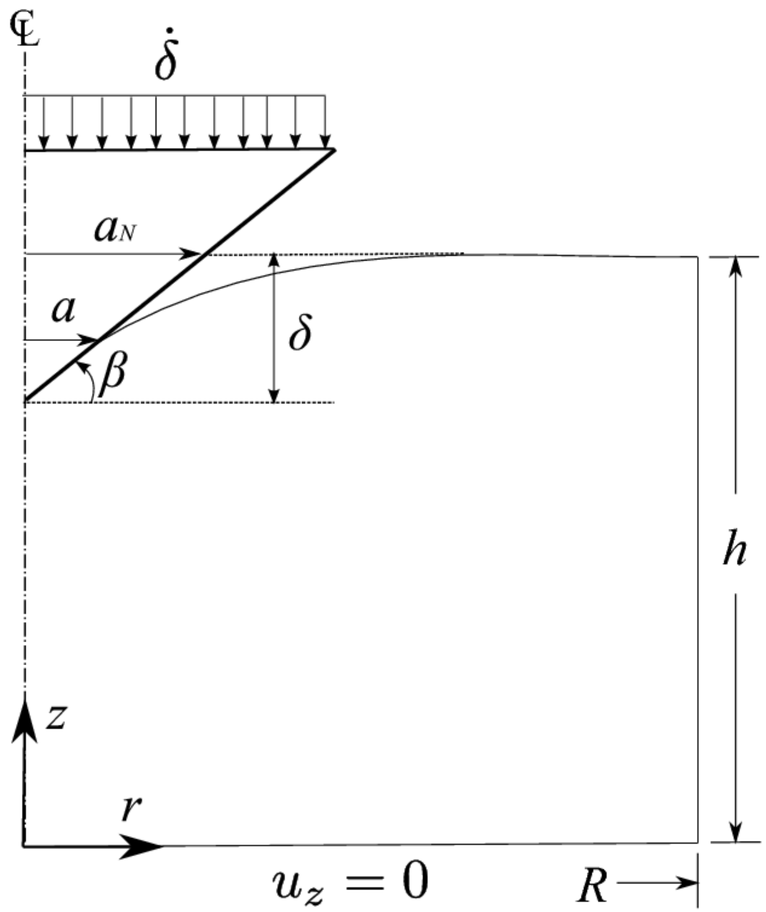
3 cases for the length scale parameters

Cases	l_1	l_2	l_3
C_1	$l_1 = l$	$l_2 = l/2$	$l_3 = \sqrt{3/8}\,l$
C_2	$l_1 = l$	$l_2 = 0$	$l_3 = 0$
C_3	$l_1 = 0$	$l_2 = l/2$	$l_3 = \sqrt{5/24}\,l$

- C_1 case corresponds to a single length scale case: $\dot{E}_p = \sqrt{\frac{2}{3}\left(\dot{\varepsilon}_{ij}^{p}\dot{\varepsilon}_{ij}^{p} + l^2\dot{\varepsilon}_{ij,k}^{p}\dot{\varepsilon}_{ij,k}^{p}\right)}$
- C_2 case stretch gradients are present (e.g., spherical expansion)
- C_3 case comprises only rotation gradients, i.e., couple-stress solid

Fleck and Hutchinson (1997)

Conical indentation setup



R : Radius of the cylinder

h : height of the cylinder

β : Effective indentation angle

a : Actual contact radius

a_N : Nominal contact radius

δ : Indentation depth

$\dot{\delta}$: Rate of indentation depth

L : Load conjugate to δ

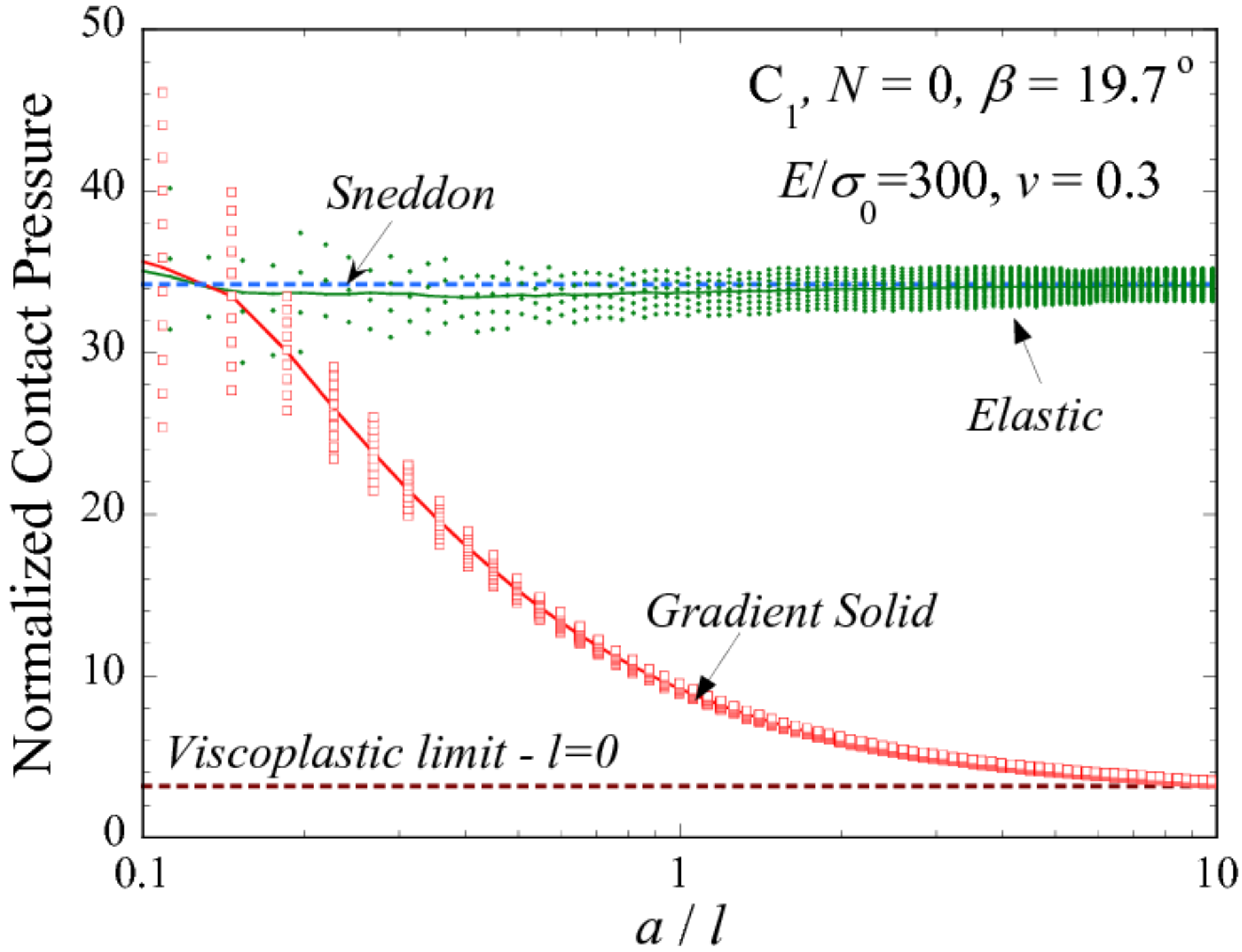
Hardness $= H = P = \dfrac{L}{\pi a^2}$ ➡ Normalized Contact Pressure $= \dfrac{P}{\sigma_0 \left(\dot{\delta} / (a\,\dot{\varepsilon}_0)\right)^m}$

Bower et al. (1993)

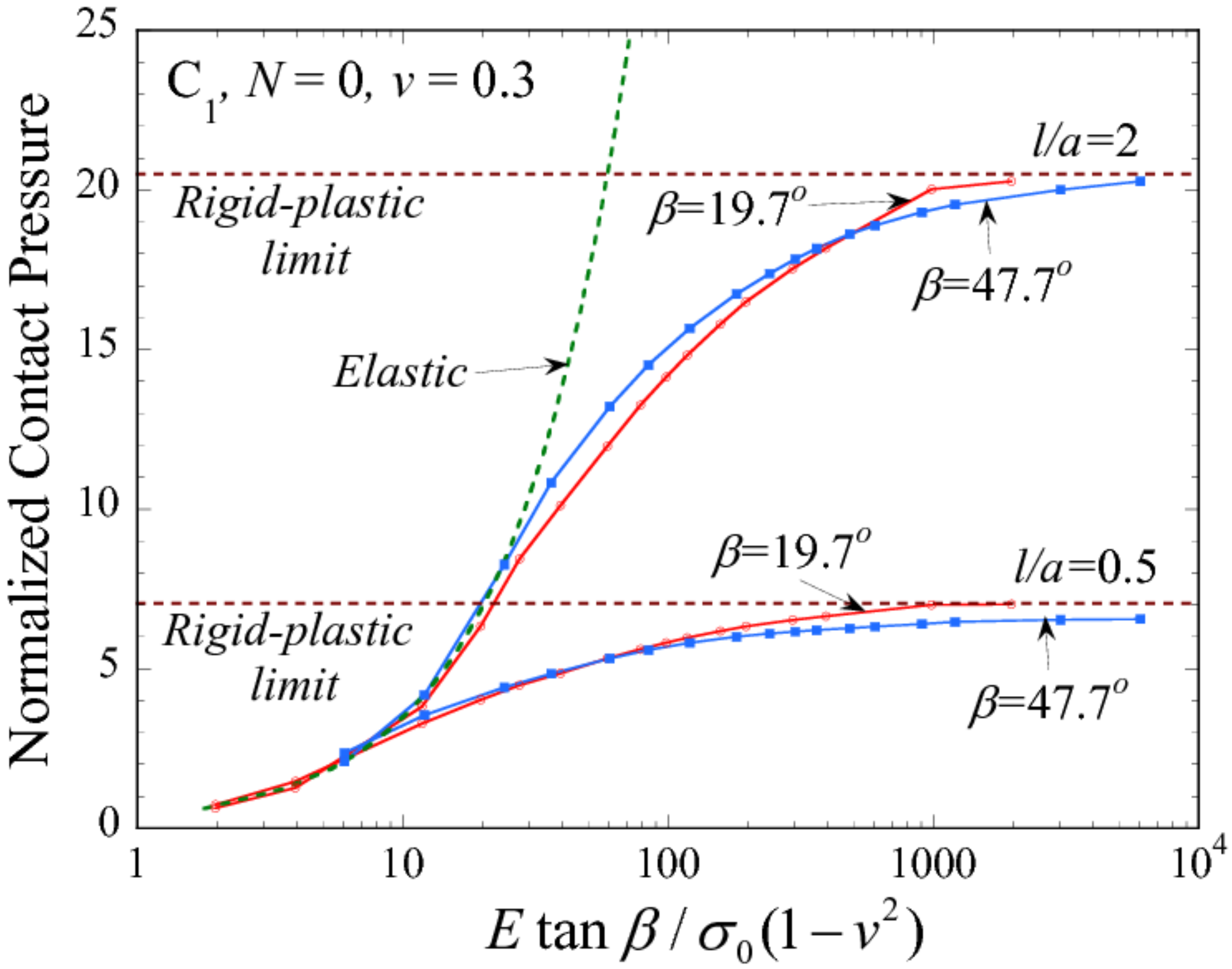
Non-hardening materials

$$N=0$$

Filling the gap between elasticity and plasticity



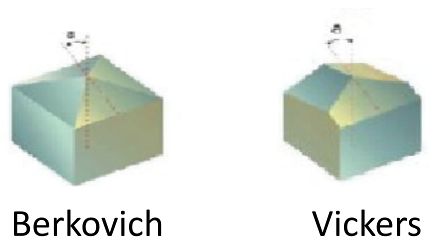
Two indenter angles



[Johnson (1970)]

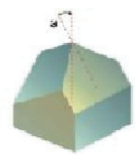
Berkovich or Vickers

$\beta = 19.7^o$



Cube corner

$\beta = 47.7^o$

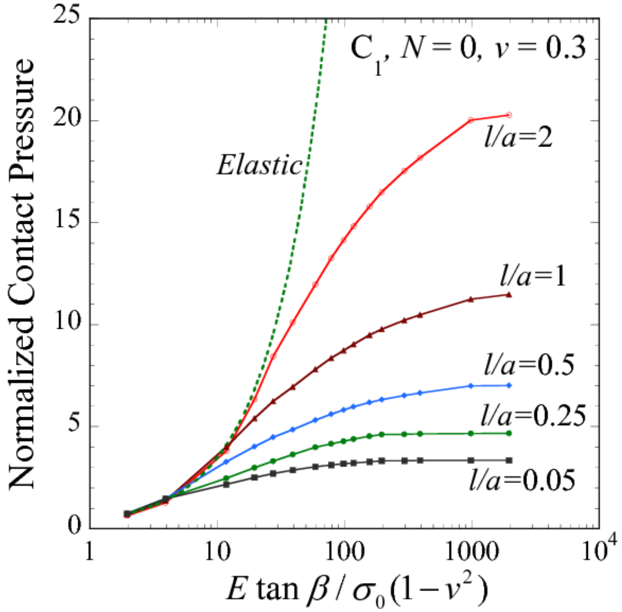


NOTE: The pressure curves comprise 3 zones: (i) elastic, (ii), elasto-plastic and (iii) rigid-plastic.

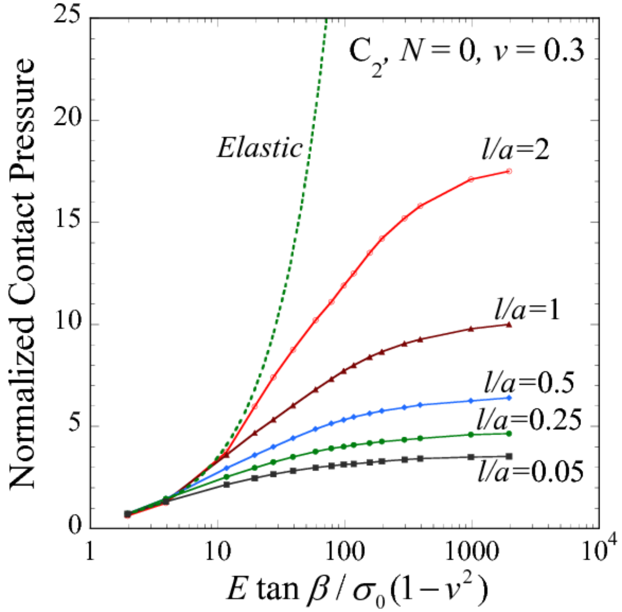
Comparison of the 3 length scales

<u>Representative Cases</u>

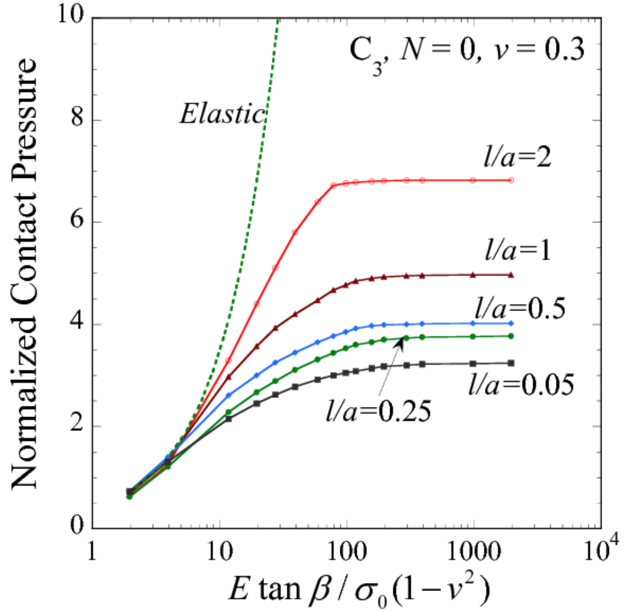
C_1



C_2

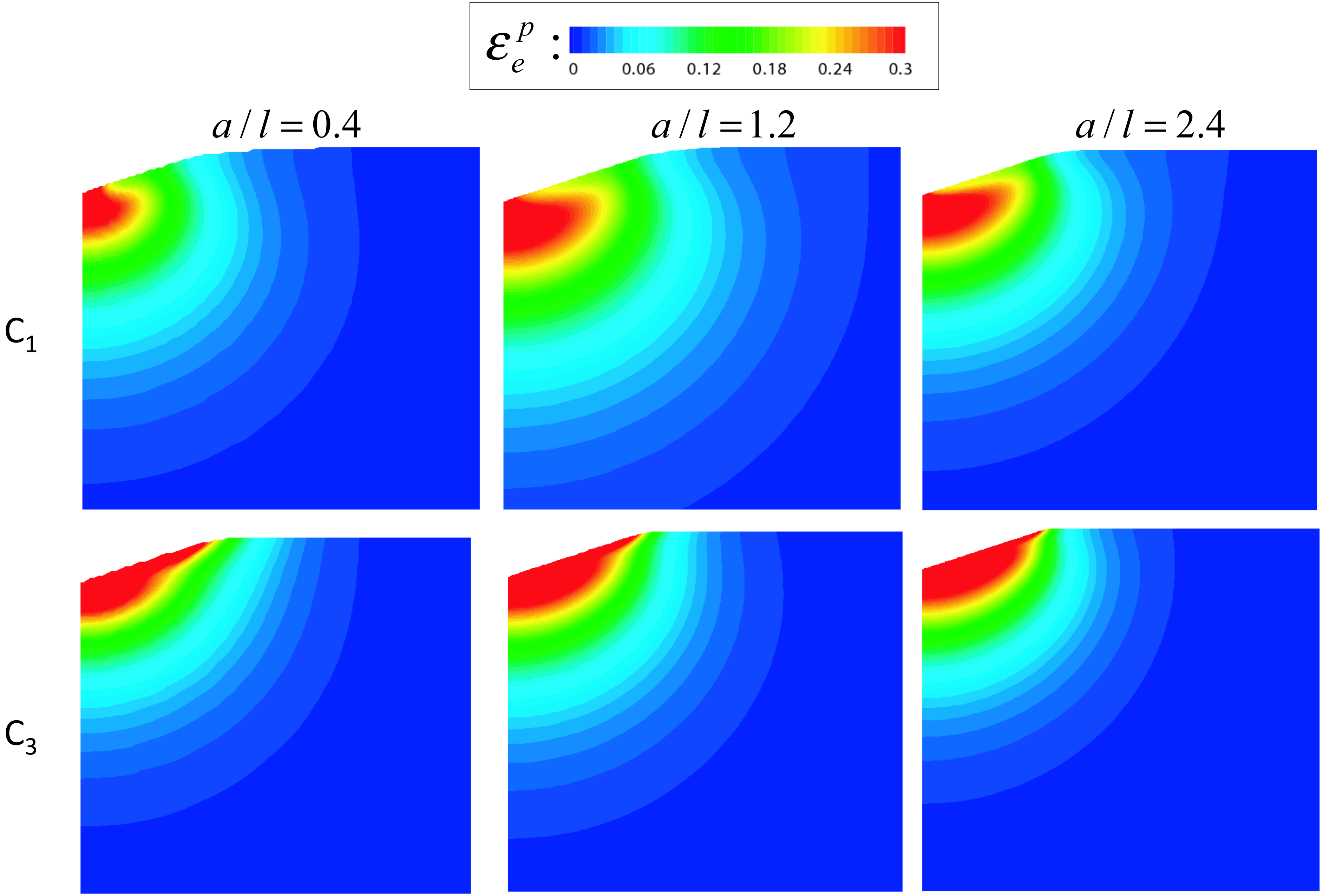


C_3



Single length scale	Stretch gradients	Rotation gradients
$l_1 = 2l_2 = \sqrt{8/3}\, l_3 = l$	$l_1 = l,\ l_2 = l_3 = 0$	$2l_2 = \sqrt{24/5}\, l_3 = l$ $l_1 = 0$

Contours of plastic strain – E/σ_0=1000



Hardening materials

Hardening materials

- Remind of Hardening law:

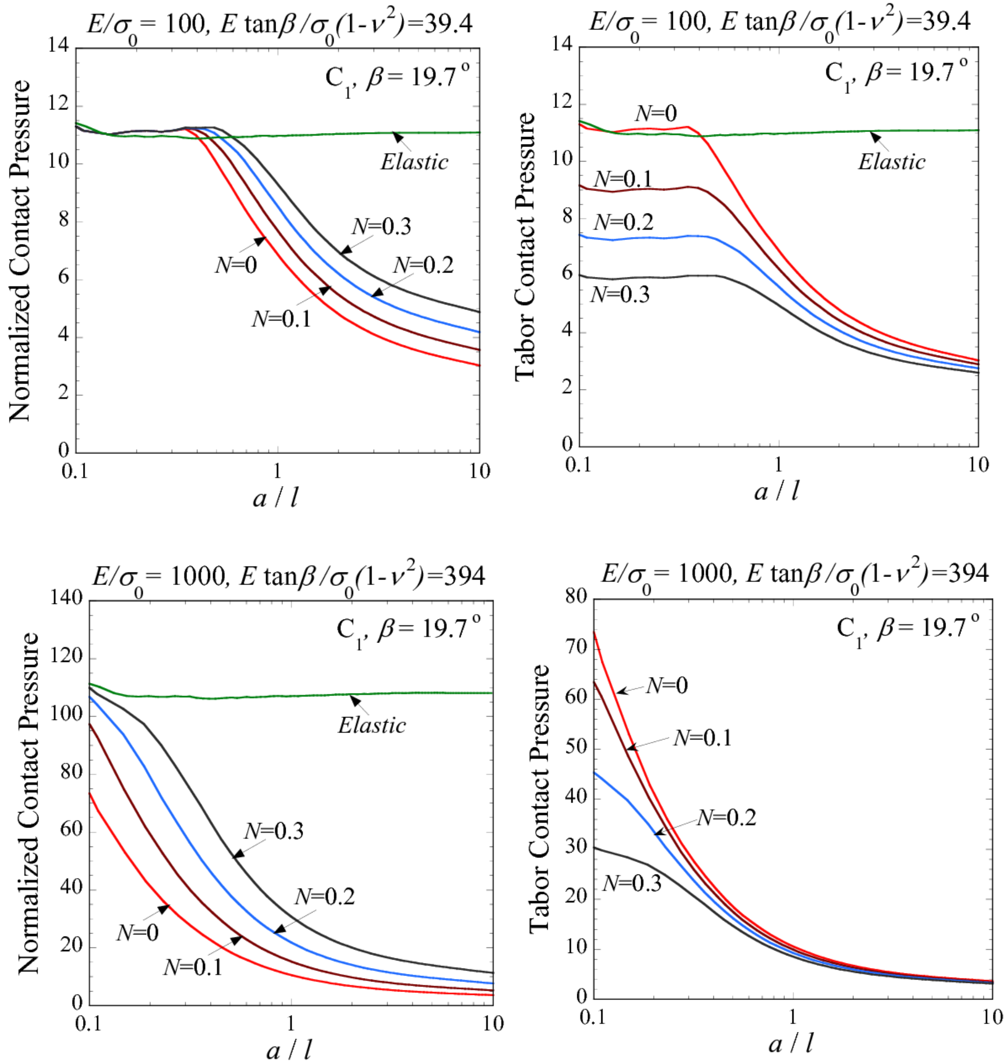
$$\sigma_y\left(E_p\right)=\sigma_0\left(1+E_p/\varepsilon_0\right)^N$$

$$\varepsilon_0=\sigma_0/E$$

- Tabor (1948) effective strain approximation

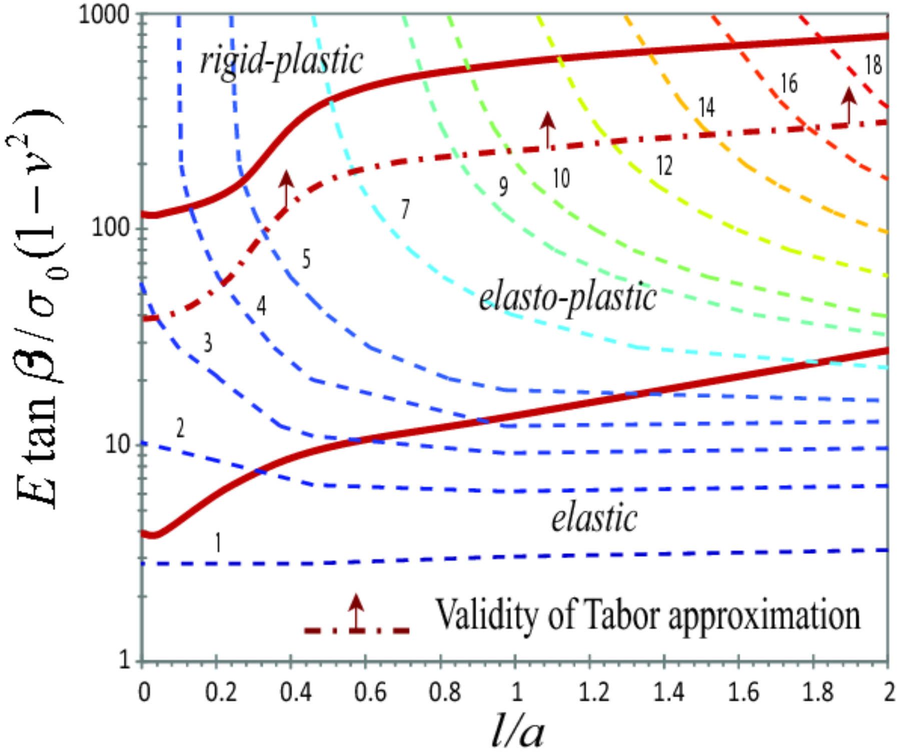
$$\sigma_{eff}=\sigma_0\left(1+\frac{\varepsilon_{eff}}{\varepsilon_0}\right)^N,\quad \varepsilon_{eff}=0.2\tan\beta$$

$$P_{Tabor}=\frac{P}{\sigma_{eff}\left(\dot{\delta}/(a\,\dot{\varepsilon}_0)\right)^m}$$

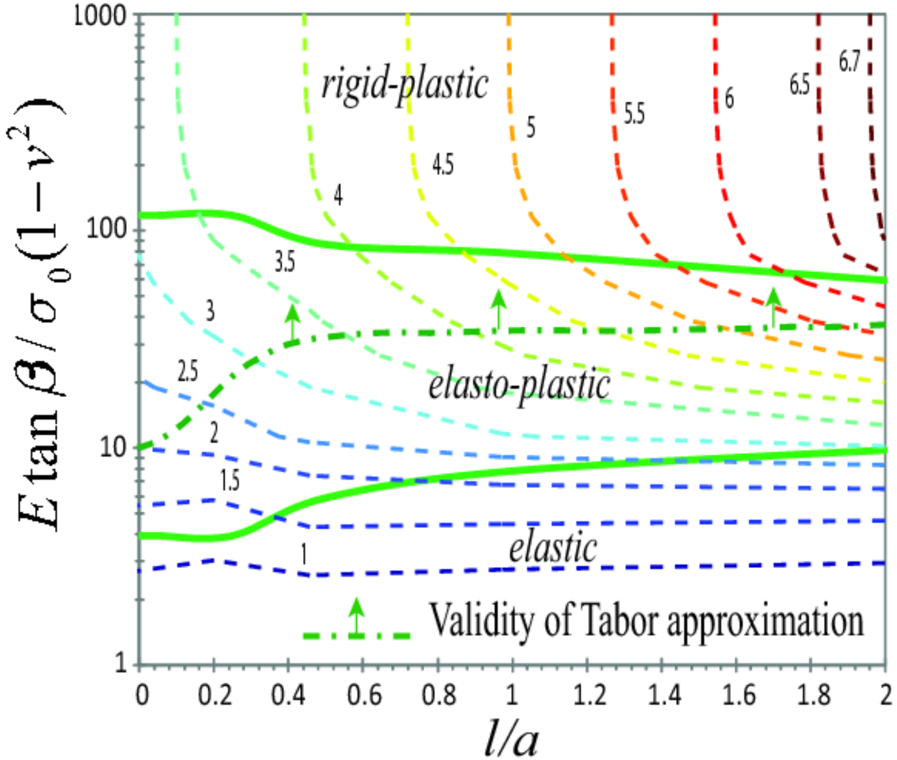


Maps showing regimes of deformation

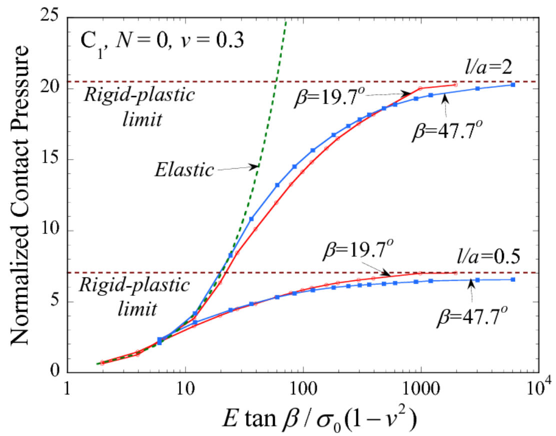
C_1



C_3



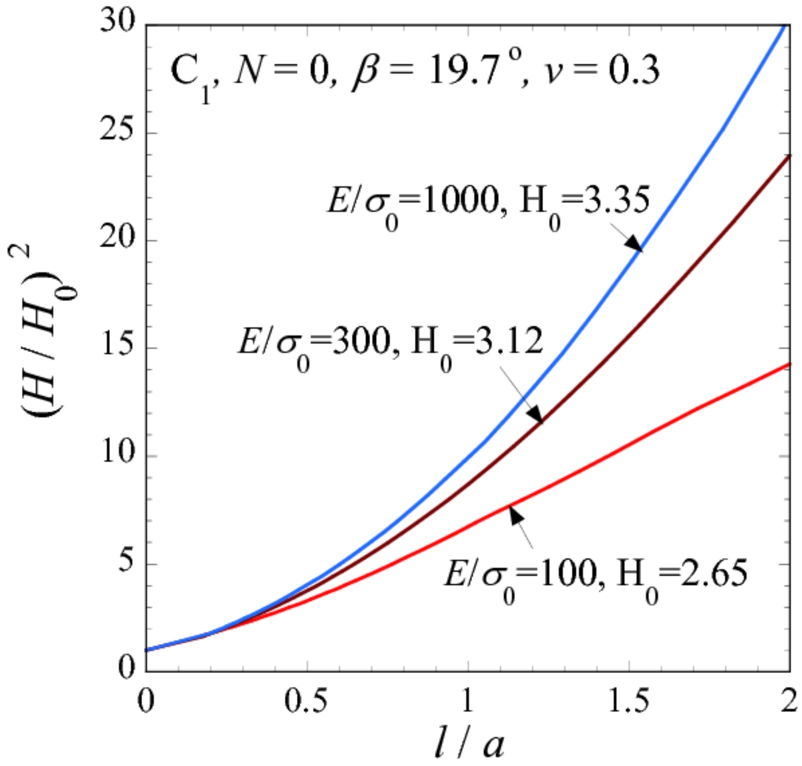
Remind

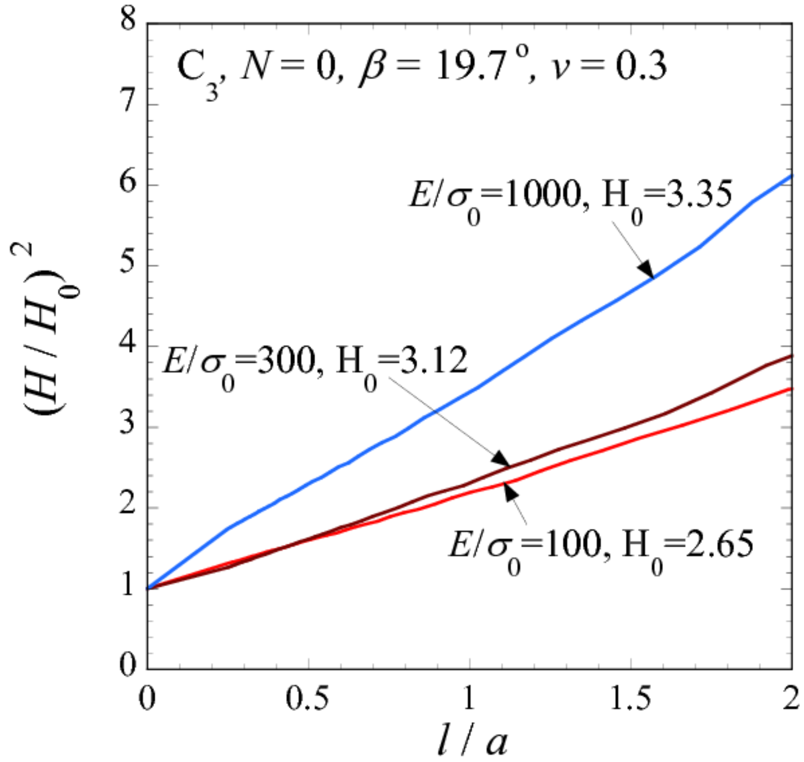


FEM results vs. Nix-Gao trends

- The Nix and Gao (1998) phenomenological formula implies:

$$\left(\frac{H}{H_0}\right)^2 \sim \frac{l}{a}$$





Concluding remarks

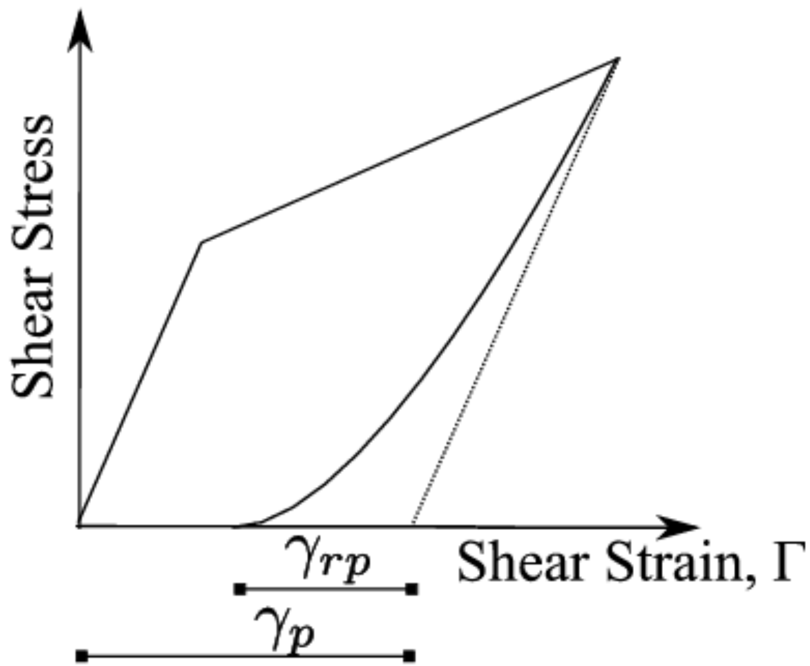
- The indentation hardness predicted by the present SGP formulation recovers first the elastic Sneddon solution, and smoothly decreases to attain the conventional large scale indentation hardness.
- The indentation hardness curves comprise 3 distinct regimes of different deformation mechanisms; (i) elastic, (ii) elasto-plastic and (iii) rigid-plastic.
- For hardening materials with low yield strain (mainly metallic materials), Tabor (1948) effective strain approximation works sufficiently well.
- The use of stretch gradients, contrary to a solid with only rotation gradients does not reproduce qualitatively the Nix & Gao experimental trends.

Thank you for

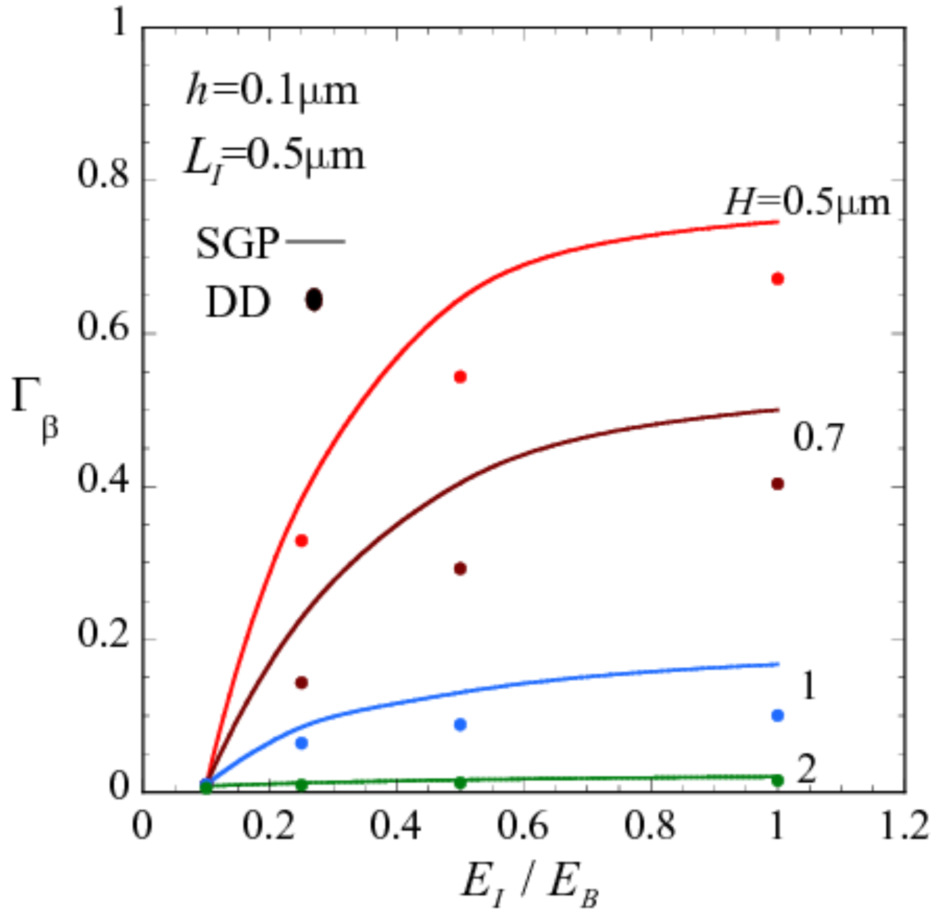
your attention!

SGP vs. DD: measure of the Bauschinger effect

$$\Gamma_\beta \in [0,1] \equiv [\text{no Bauschinger effect, no dissipation}]$$



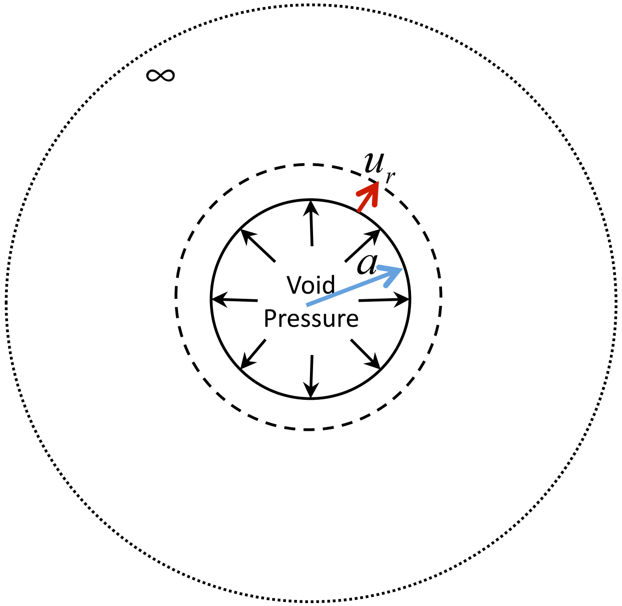
$$\Gamma_\beta = \gamma_{rp}/\gamma_p$$

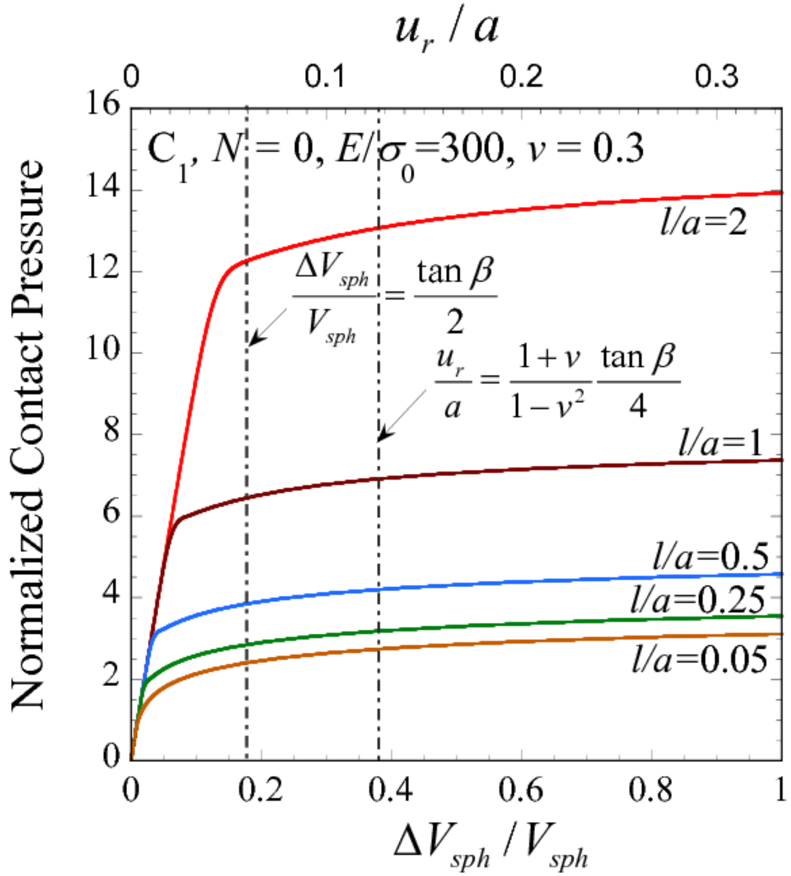


Evaluation of other models

Spherical expansion of a void

$$l_1 = 2l_2 = \sqrt{8/3}\, l_3 = l$$





- Johnson(1970), Wei & Hutchinson (2003)

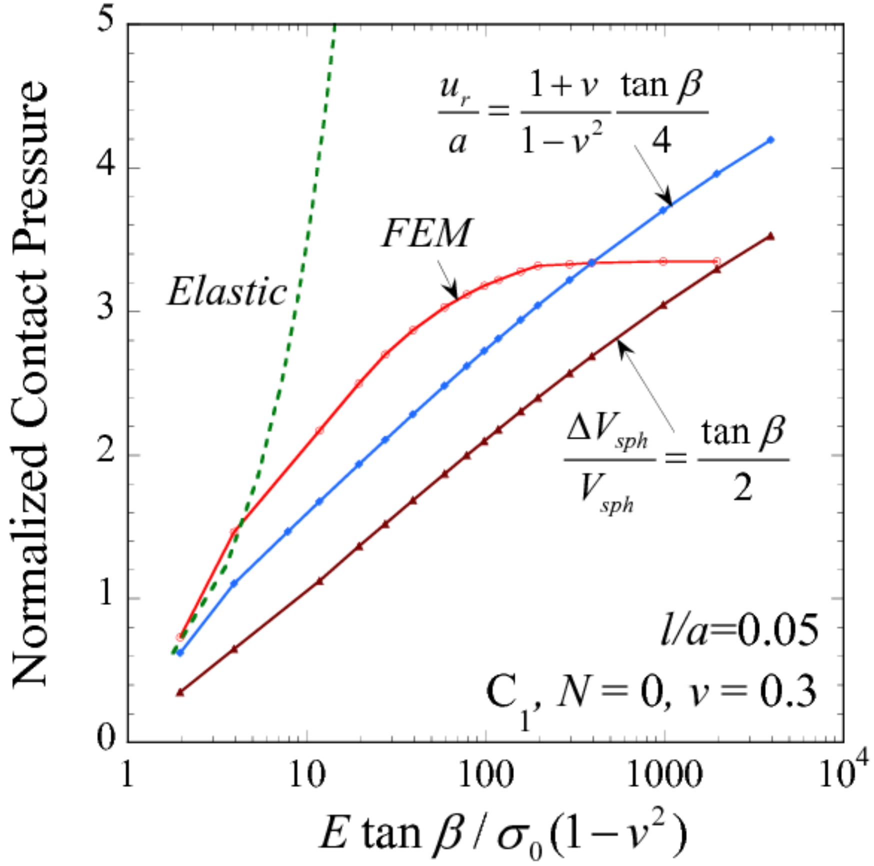
$$\frac{\Delta V_{sph}}{V_{sph}} = \frac{\tan\beta}{2} \Rightarrow \boxed{\frac{u_r}{a} = \frac{\tan\beta}{6}}$$

- Solving the purely elastic problem

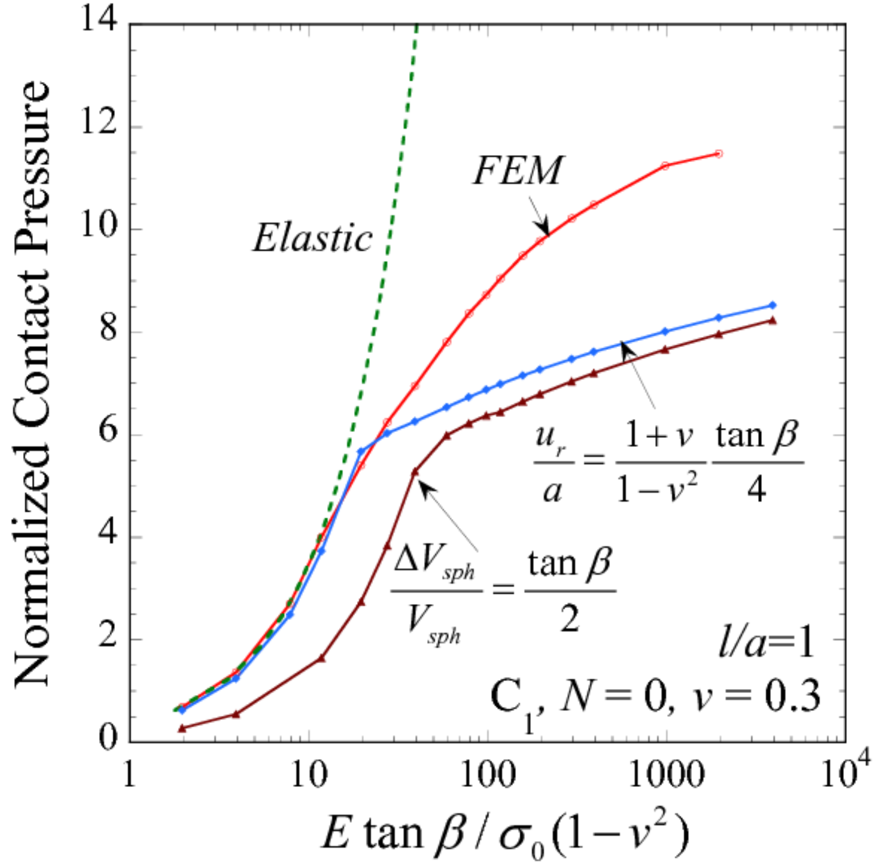
$$P_{sneddon} = \frac{E}{1-\nu^2}\frac{\tan\beta}{2} \equiv P_{sph} = \frac{2E}{1+\nu}\frac{u_r}{a} \Rightarrow \boxed{\frac{u_r}{a} = \frac{1+\nu}{1-\nu^2}\frac{\tan\beta}{4}}$$

Spherical expansion vs. FEM results

Large scales, l/a=0.05

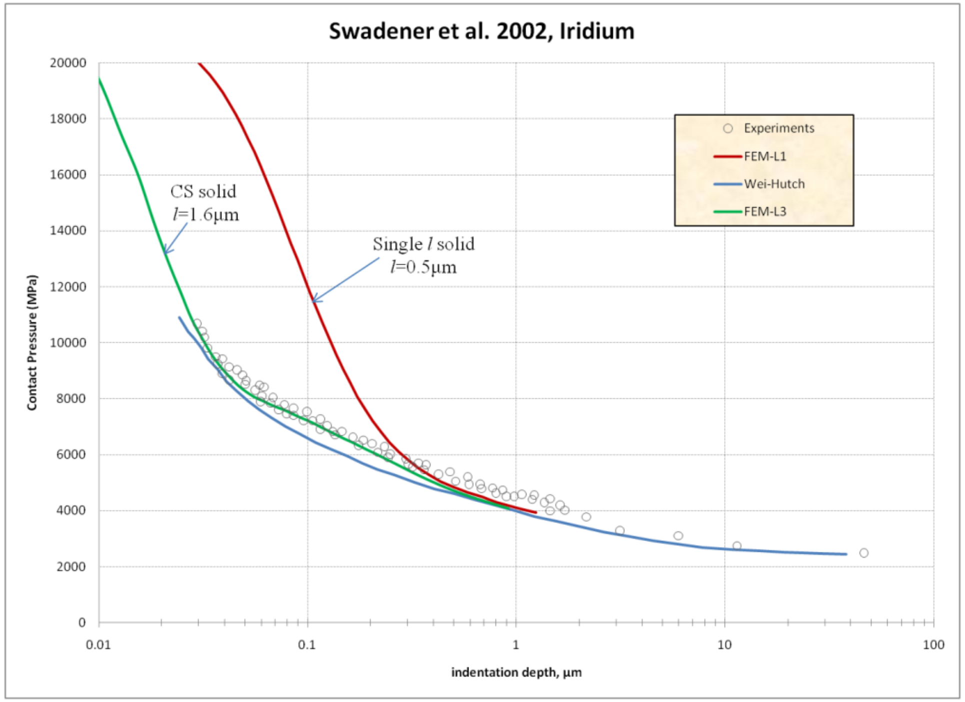


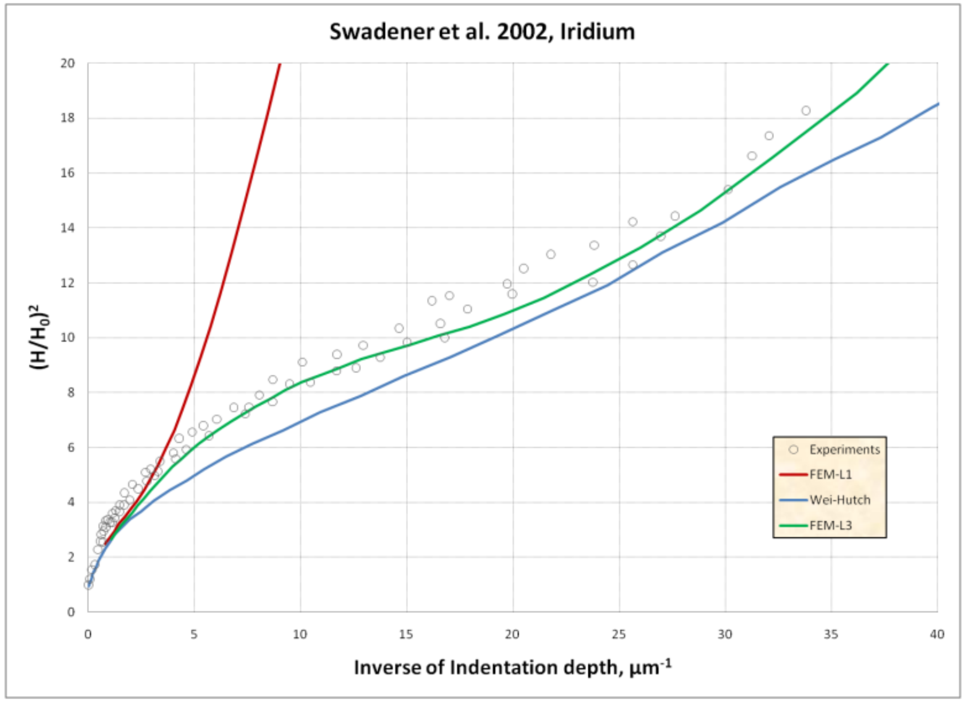
Micron scales, l/a=1



- NOTE: In his original results, Johnson (1970) used a correction term in the computed void pressure to have a better fit in the experiments. The above results are without this term.

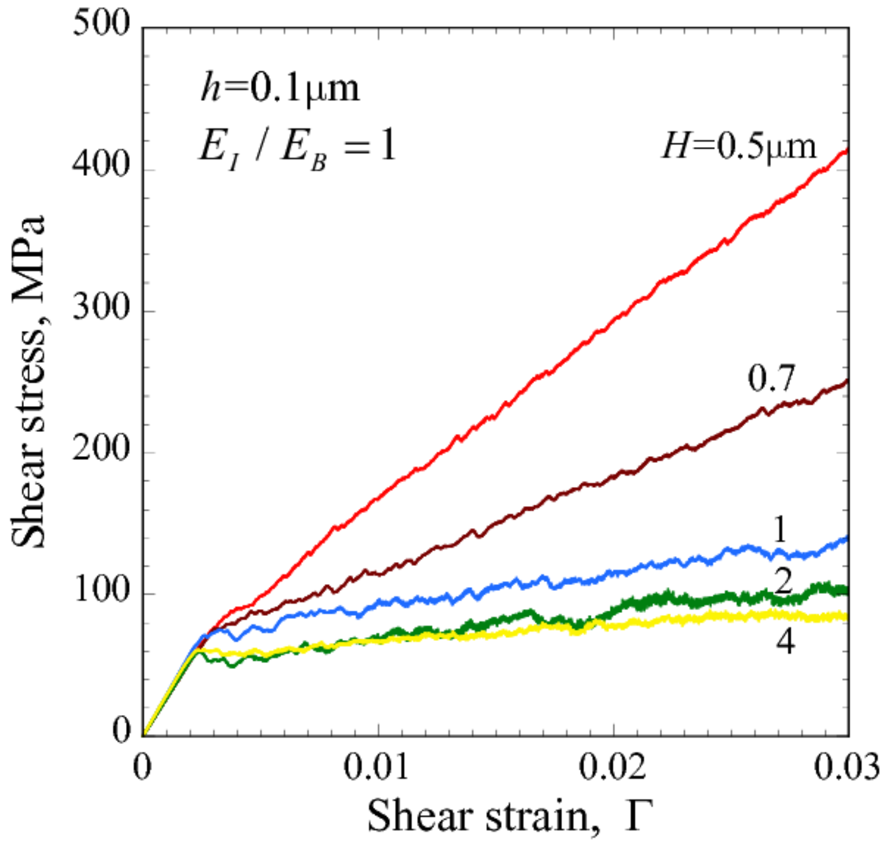
Preliminary experimental results

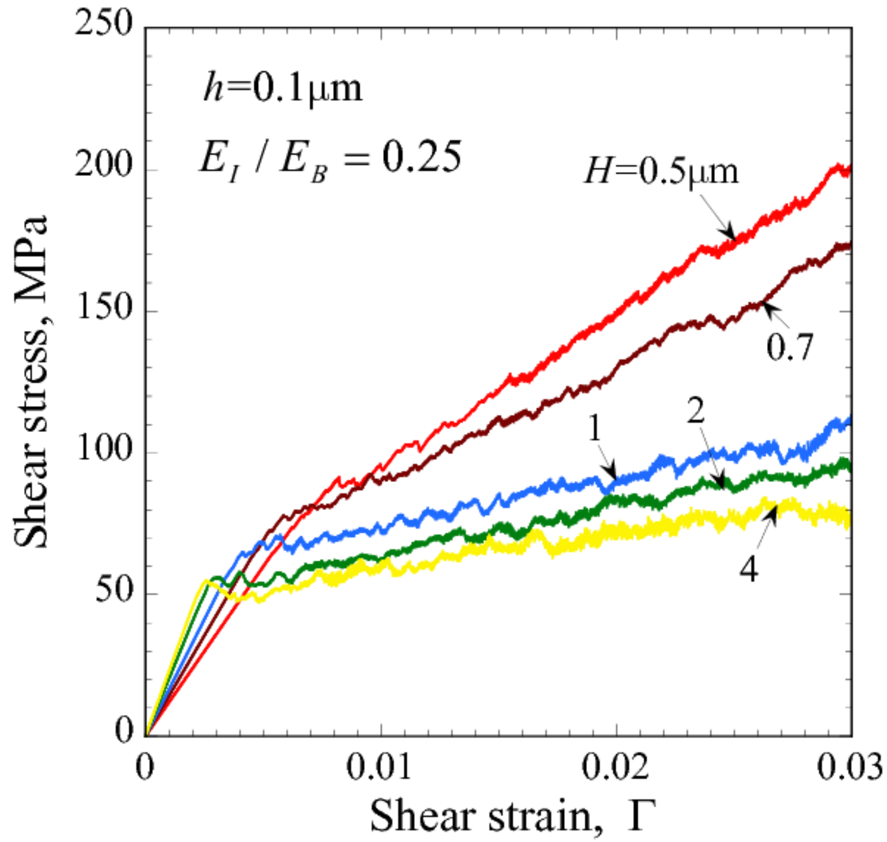




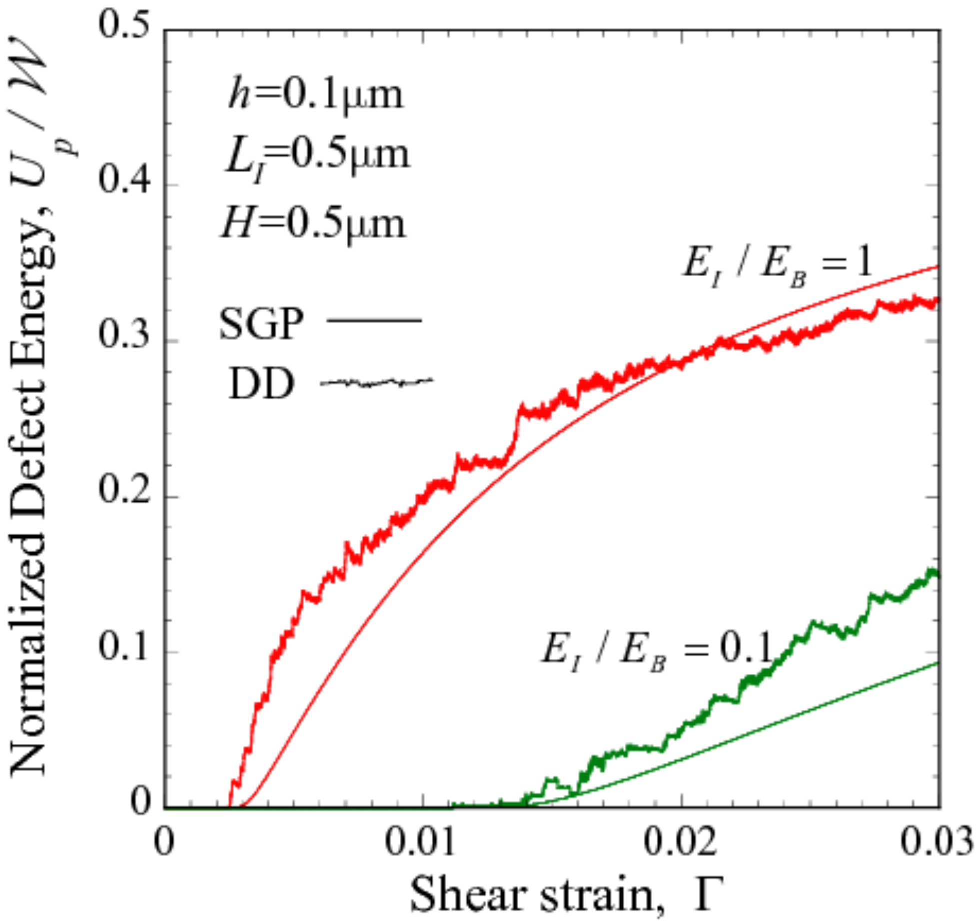
DD Shear Stress results

Sensitivity analysis of the height of the crystal H





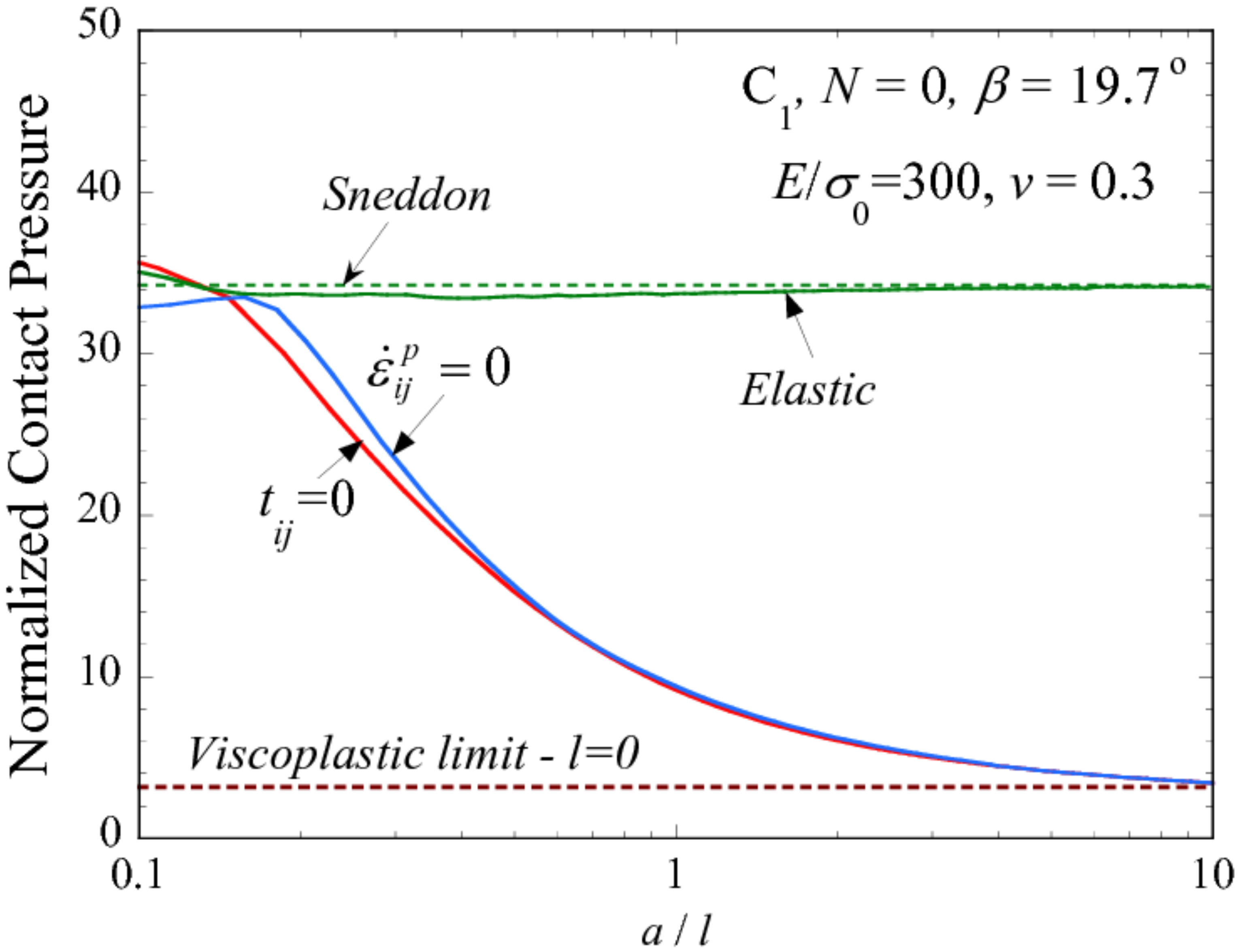
SGP vs. DD: defect energy over work done



U_p : is the defect energy due to the presence of the GNDs

$\mathcal{W}$: is the total work done by the external forces

Effect of BC's in conical indentation



Size effects in polycrystals

Hall-Petch law : $\sigma = \sigma_0 + k\, d^{-1/2}$