A Unified Theory for Modeling Damage to Real Surfaces in Contact

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Aerospace

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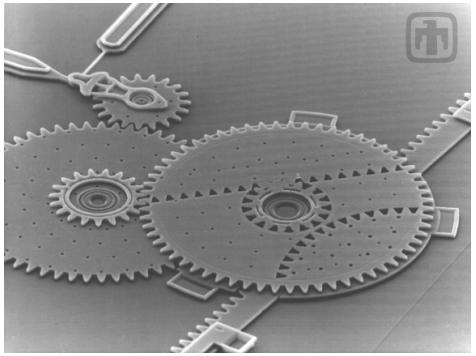


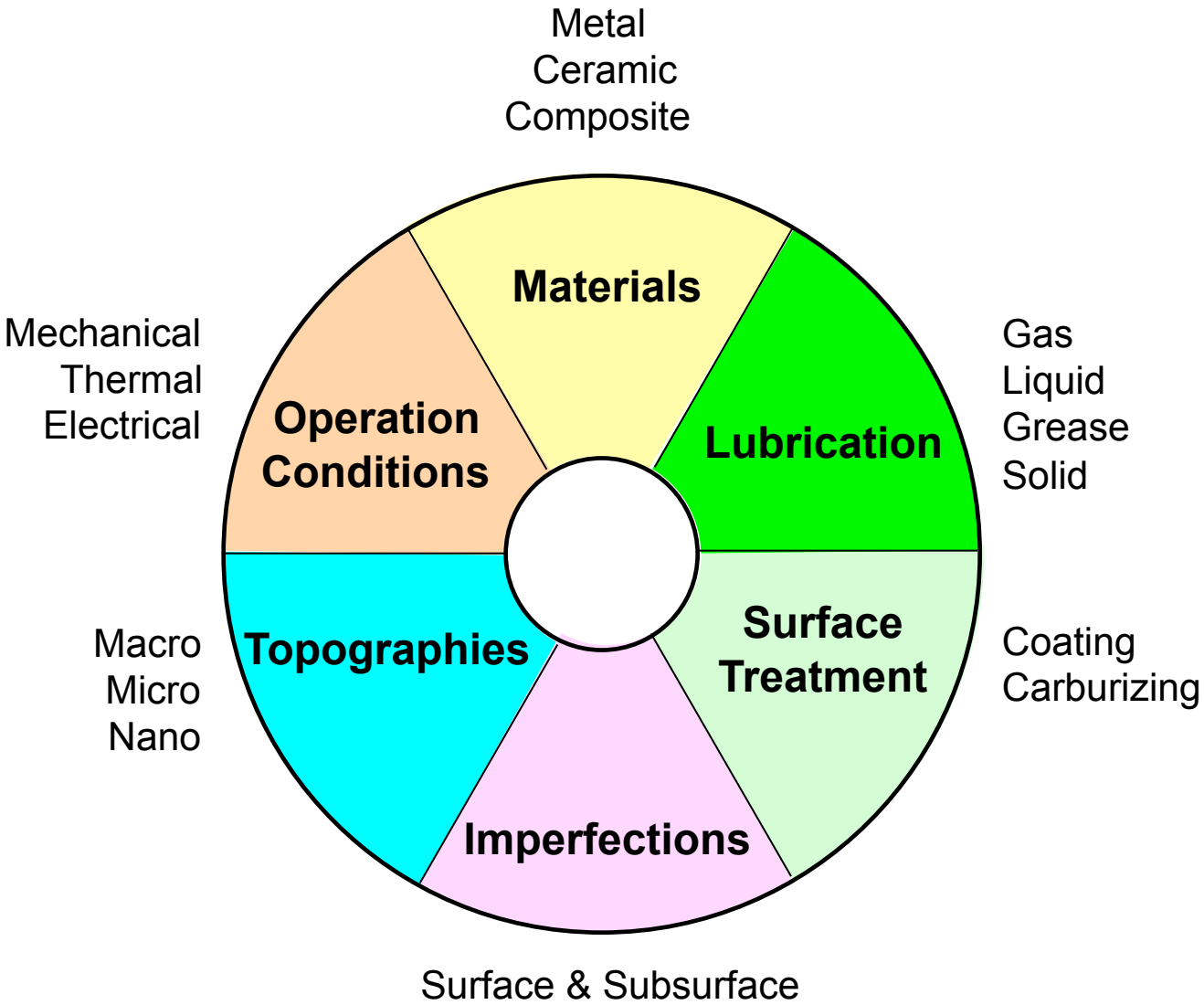
Sandia National Laboratory, USA

"In highly industrialized nations, the total annual cost of **friction-and wear-related energy and material losses** is estimated to be **5 % - 7% of national gross domestic product (GDP)**…"

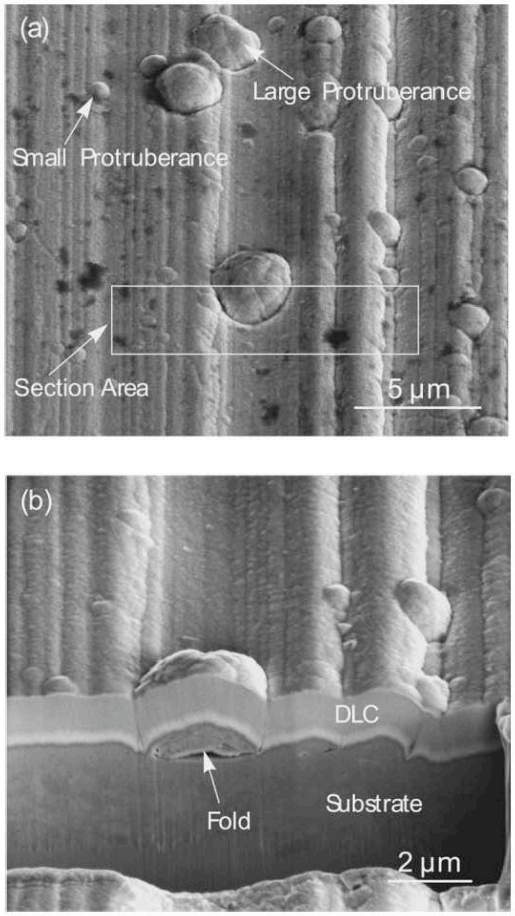
– U.S. Department of Energy, June 2009

(The 2008 US GDP was **$ 14.2 trillion** according to World Bank data)

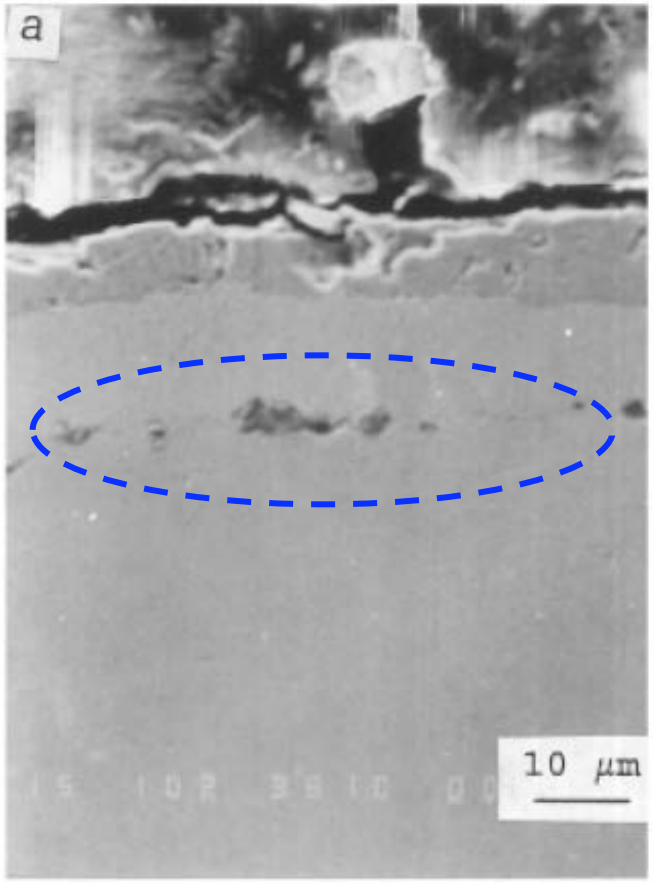
Factors Affecting Surface Performance



Surface & Subsurface Imperfections



Nodules in a diamond-like carbon (DLC) film on steel (Wang *et al.*, 2002)

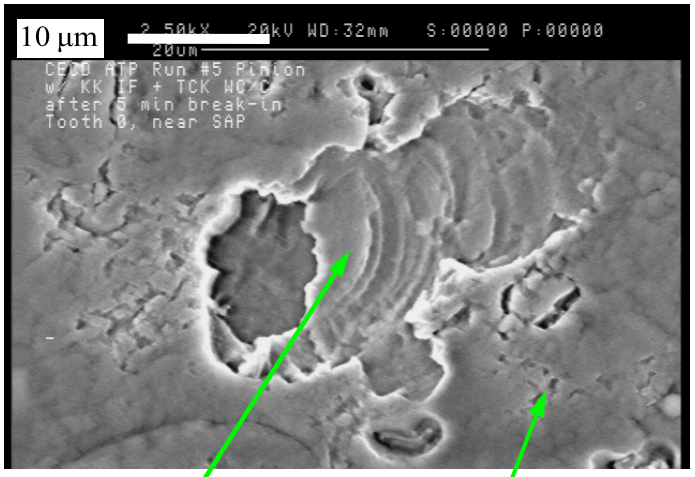


A stringer of aluminum oxides in steel (Ray *et al.*, 1999)

Surface Damage

- Particle pull-out
- Chipping wear (remove material through cracking)
- Gradual wear (gradually remove material through cyclic contact)
- Plastic deformation

Particle pull-out



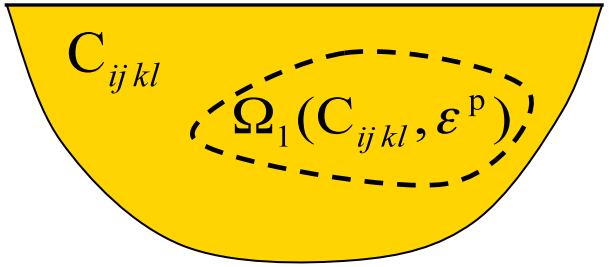
chipping wear

Gradual wear

Surface damage on tungsten diamond-like carbon (W-DLC) coatings
(Caterpillar Inc., USA)

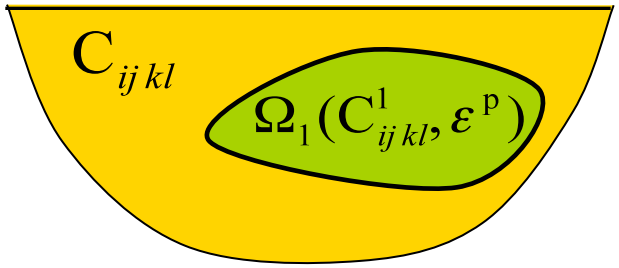
Terminology

- **Homogeneous inclusion (Mura, 1987)**
  - — same material as the matrix
  - — with eigenstrain ε^{p}



Eigenstrain: inelastic strain such as thermal strain, plastic strain, etc.

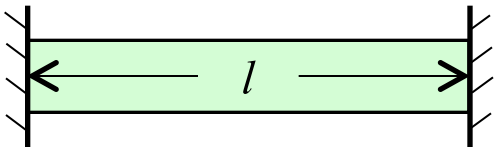
- **Inhomogeneous inclusion**
  - — different material than the matrix ($C^{1}_{ijkl} \neq C_{ijkl}$)
  - — with/without eigenstrain *



(e.g., voids, nonmetallic oxides in steel, and fibers/particles in composites)

* Researchers also use “inhomogeneity” to term an inhomogeneous inclusion without eigenstrain.

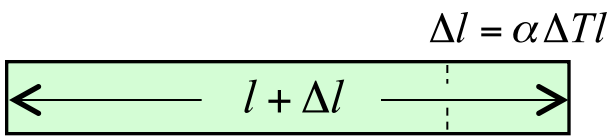
Eigenstrain: A Sample Illustration



Total strain: $\varepsilon = 0$

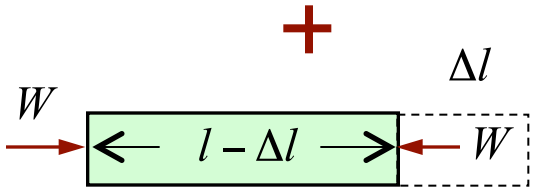
Temperature raised by ΔT in a constrained 1D bar

α : linear coefficient of thermal expansion



Free thermal expansion

Eigenstrain: $\varepsilon^{\mathrm{p}} = \alpha \Delta T$



Mechanical deformation

Elastic strain: $\varepsilon^{\mathrm{e}} = -\alpha \Delta T$

$$\varepsilon = \varepsilon^{\mathrm{p}} + \varepsilon^{\mathrm{e}} = 0$$

Stress: $\sigma = E\varepsilon^{\mathrm{e}} = -E\alpha\Delta T$ (Hooke's law)

Previous Theoretical Studies

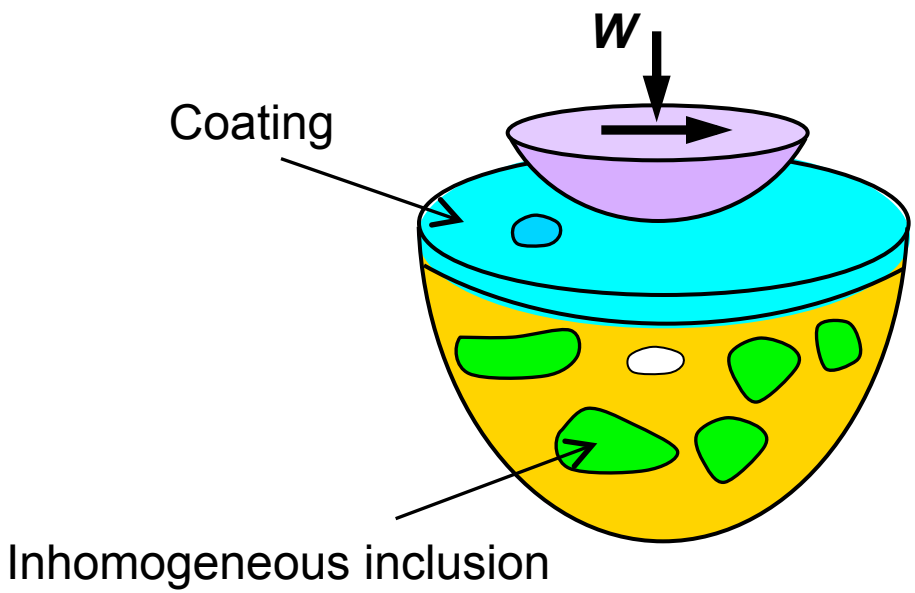
- **Inhomogeneous inclusions in an infinite space (3D)**
  - Single (most studied) e.g., Eshelby, 1957
  - Two (few studied) e.g., Moschovidis & Mura, 1975

- **Inhomogeneous inclusions near surfaces (3D)**
  - Single (few studied) e.g., Kouris & Mura, 1989
  - Two (very few studied) e.g., Molchanov *et al.,* 2002

- **Inhomogeneous inclusions near surfaces in contact (2D)**
  - Single (Miller & Keer, 1983; Kuo, 2007)
  - Multiple (Kuo, 2008)

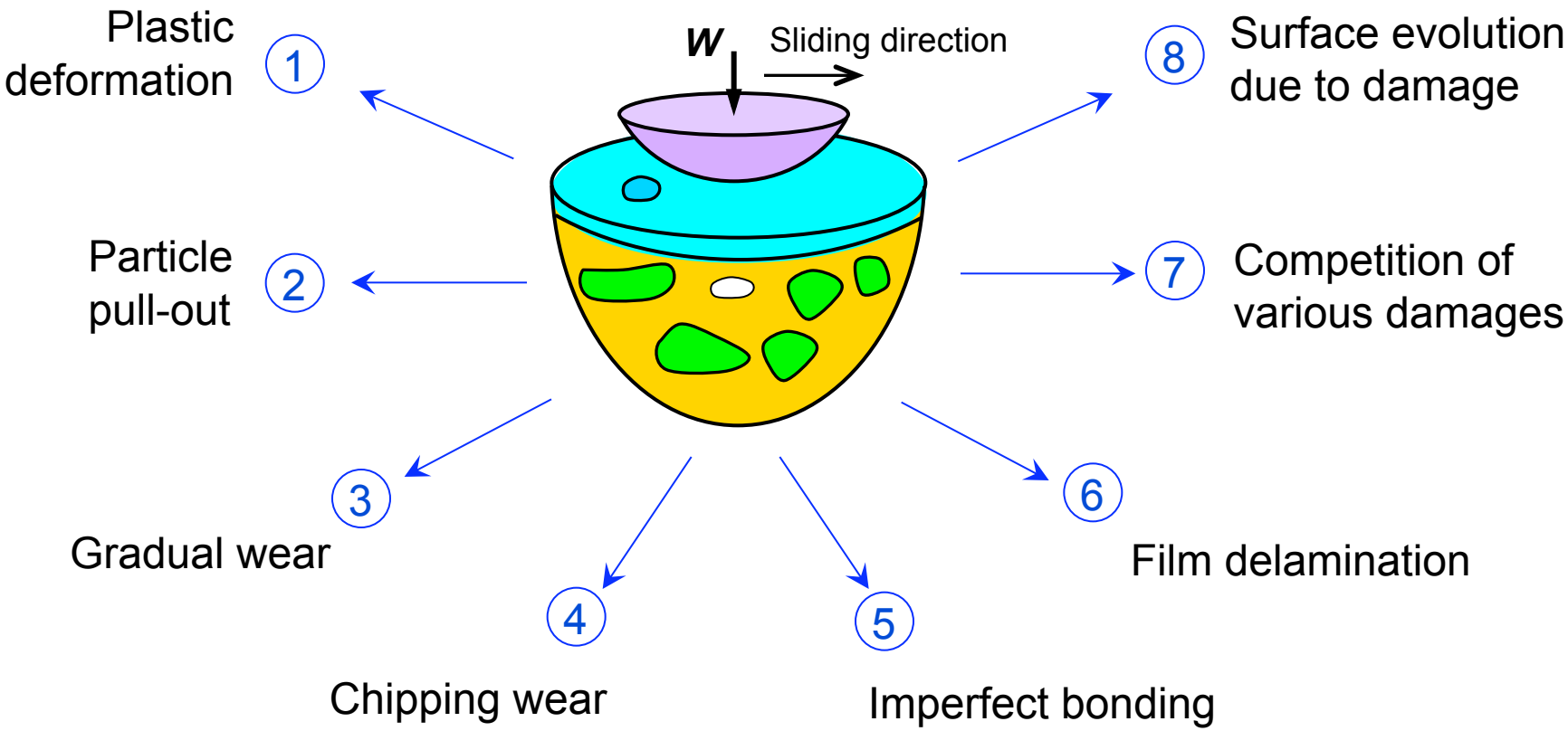
Research Goals

- Model multiple inhomogeneous inclusions of 3D arbitrary shape near surfaces in contact.
- Address challenging surface problems involving material dissimilarity and inelastic deformation.



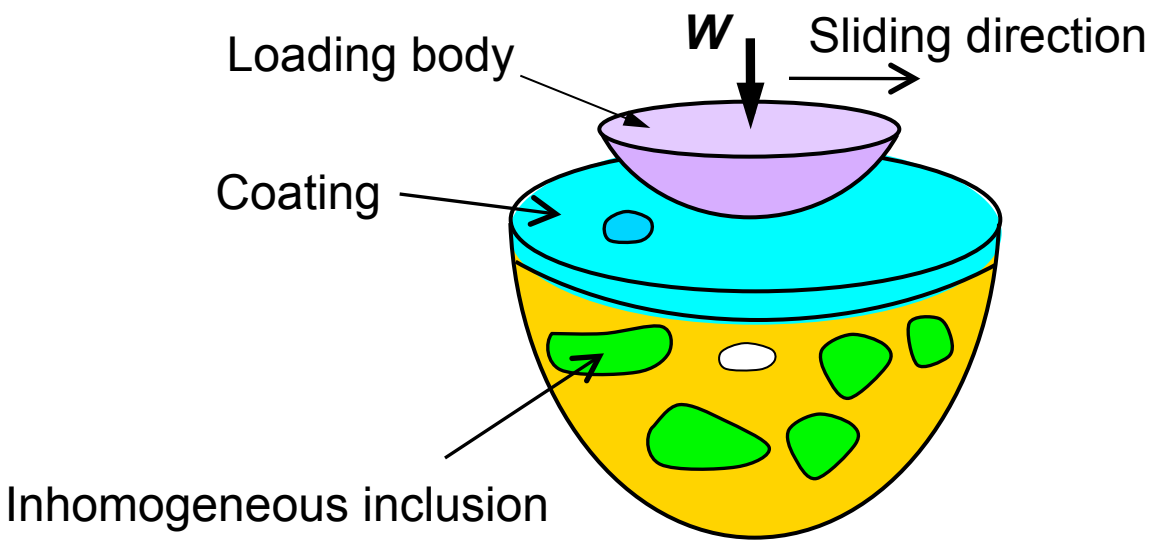
Research Goals

- Develop a unified theory to model damage to real surfaces in contact.



Research Challenges

- Account for material dissimilarity
- Model interactions between the inclusions, coating, and loading body
- Determine contact pressure and contact area
- Expand the theory to predict various damages



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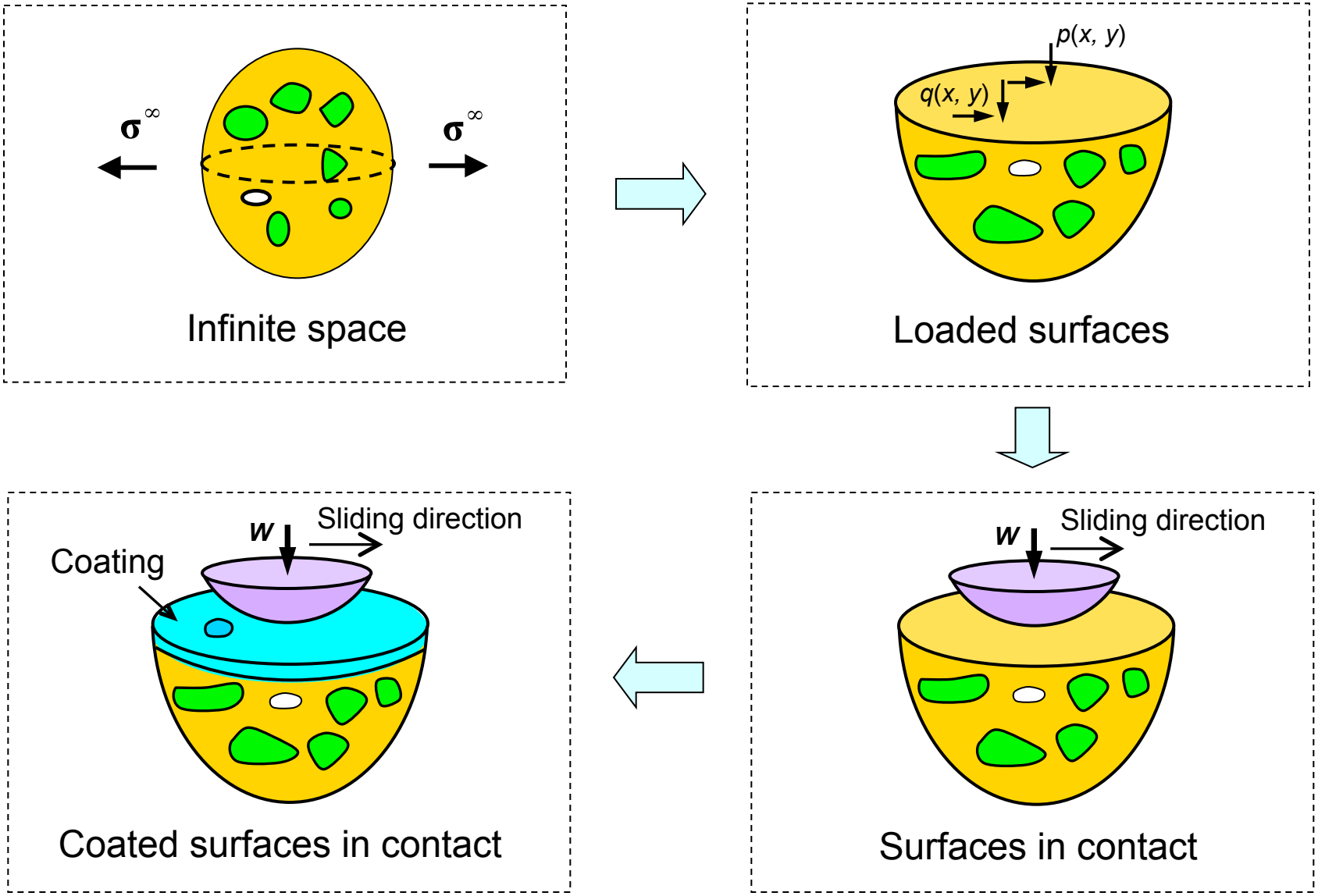
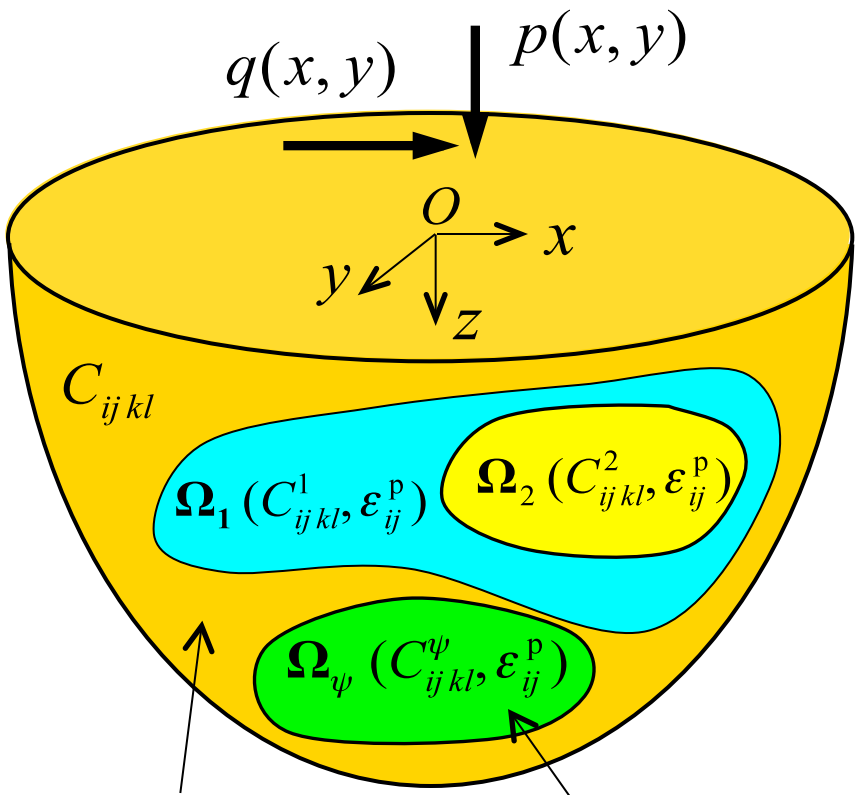
Models Developed in Research



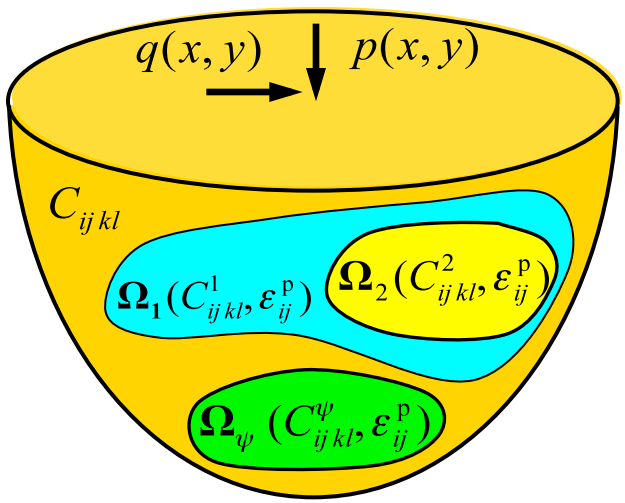
Inhomogeneous Inclusions Near Surfaces



Generality

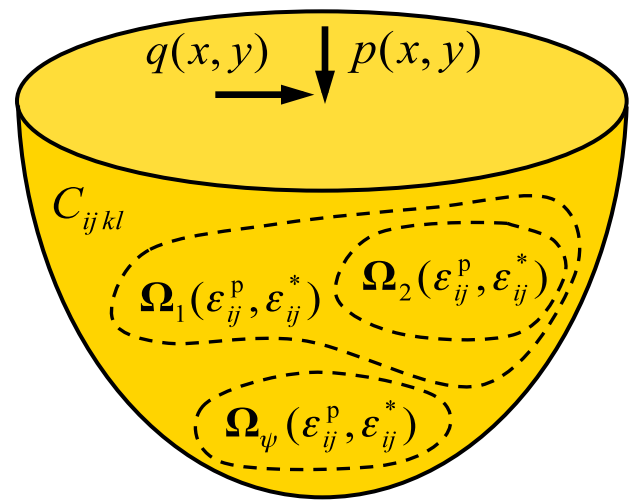
- 3D arbitrary shape
- Multiple number
- Various materials
- Full interactions
- Non-uniform initial eigenstrain $\varepsilon^{\mathrm{p}}_{ij}$

Equivalent Inclusion Method: an inhomogeneous inclusion is treated as a homogenous inclusion with initial eigenstrain $\varepsilon_{ij}^{\mathrm{p}}$ plus equivalent eigenstrain ε_{ij}^{*} (Eshelby, 1957) .



Hooke's law : $\sigma_{ij} = C^{\Psi}_{ijkl}(\varepsilon_{kl} - \varepsilon^{\mathrm{p}}_{kl})$ (1)

=



Hooke's law: $\sigma_{ij} = C_{ijkl}(\varepsilon_{kl} - \varepsilon^{\mathrm{p}}_{kl} - \varepsilon^{*}_{kl})$ (2)

Decomposition: $\sigma_{ij} = \sigma^{*}_{ij} + \sigma^{\mathrm{p}}_{ij} + \sigma^{0}_{ij}$ (3)

Unknown equivalent eigenstrains ε_{ij}^{*} depend on:

- Materials
- Interactions
- External loading (initial eigenstrains & surface tractions)

Eqs.(1)-(3)

Governing Equation

$$\mathbf{C}^{\psi}\mathbf{C}^{-1}\boldsymbol{\sigma}^{*} - \boldsymbol{\sigma}^{*} + \mathbf{C}^{\psi}\boldsymbol{\varepsilon}^{*} = (\boldsymbol{\sigma}^{\mathrm{p}} + \boldsymbol{\sigma}^{0}) - \mathbf{C}^{\psi}\mathbf{C}^{-1}(\boldsymbol{\sigma}^{\mathrm{p}} + \boldsymbol{\sigma}^{0}) \qquad (4)$$

Unknowns $\boldsymbol{\varepsilon}^{*}$

Eq. (4) is not solvable until we determine:

- Eigenstress-eigenstrain relationship (solution for homogenous inclusions)

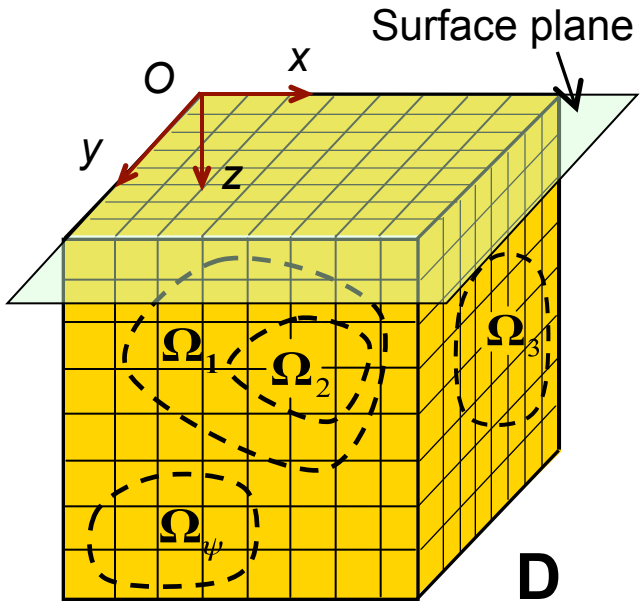
  $\boldsymbol{\sigma}^{*}$ is expressed in terms of $\boldsymbol{\varepsilon}^{*}$; $\boldsymbol{\sigma}^{\mathrm{p}}$ is expressed in terms of $\boldsymbol{\varepsilon}^{\mathrm{p}}$

- Stresses due to normal and tangential tractions at the surface

  $\boldsymbol{\sigma}^{0} \longleftarrow p(x,y)$ and $q(x,y)$

Eigenstress-Eigenstrain Relationship (Solution for Homogeneous Inclusions $\mathbf{\Omega}_\psi$)

Discretization method: each $\mathbf{\Omega}_\psi$ is approximated by many small cuboids.



$N_x \times N_y \times N_z$ cuboids in domain D

- **Uniform eigenstrain in each cuboid**
- **Non-uniform eigenstrain in each $\mathbf{\Omega}_\psi$**

Solution by superposition (Chiu, 1978; Zhou *et al*., 2009)

$$\sigma^{P}_{\alpha,\beta,\gamma} = \sum_{\varphi=0}^{N_x-1}\sum_{\psi=0}^{N_y-1}\sum_{\xi=0}^{N_z-1} \Lambda_{\alpha-\varphi,\beta-\psi,\gamma-\xi}\, \varepsilon^{P}_{\varphi,\psi,\xi} \qquad (5)$$

$$\sigma^{T}_{\alpha,\beta,\gamma} = \sum_{\varphi=0}^{N_x-1}\sum_{\psi=0}^{N_y-1}\sum_{\xi=0}^{N_z-1} \Lambda_{\alpha-\varphi,\beta-\psi,\gamma-\xi}\, \varepsilon^{T}_{\varphi,\psi,\xi} \qquad (6)$$

$$(0 \le \alpha \le N_x - 1,\ 0 \le \beta \le N_y - 1,\ 0 \le \gamma \le N_z - 1)$$

Solution Evaluation and Validation

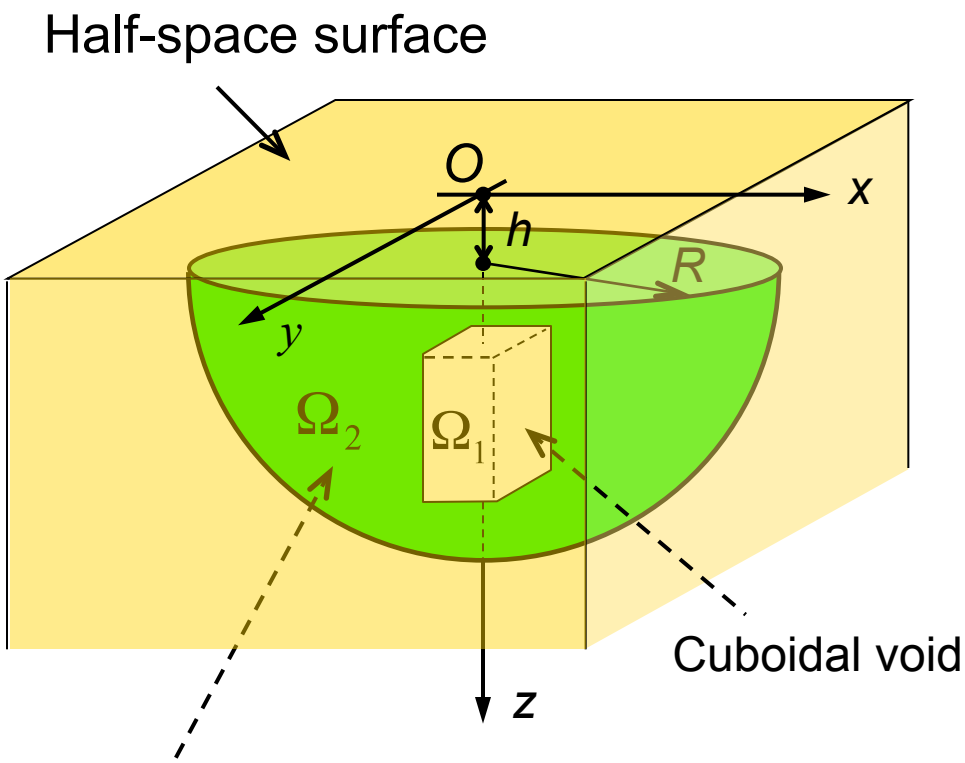
Numerical Algorithms

- Conjugate Gradient Method-based algorithm to determine unknown equivalent eigenstrains
- Fast Fourier transform algorithm to improve computational efficiency

Approach validation

- A single ellipsoidal inhomogeneous inclusion in an infinite space (Eshelby, 1957)
- Two interacting ellipsoidal inhomogeneous inclusions in an infinite space (Shodja & Sarvestani, 2001)

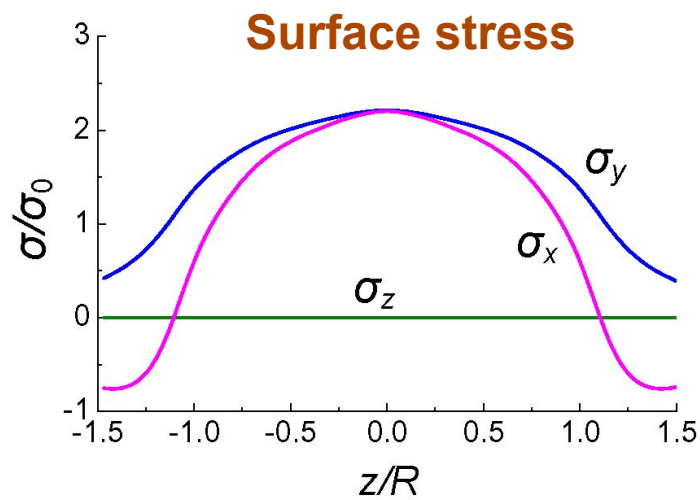
A Cuboid Void in an Inhomogeneous Inclusion

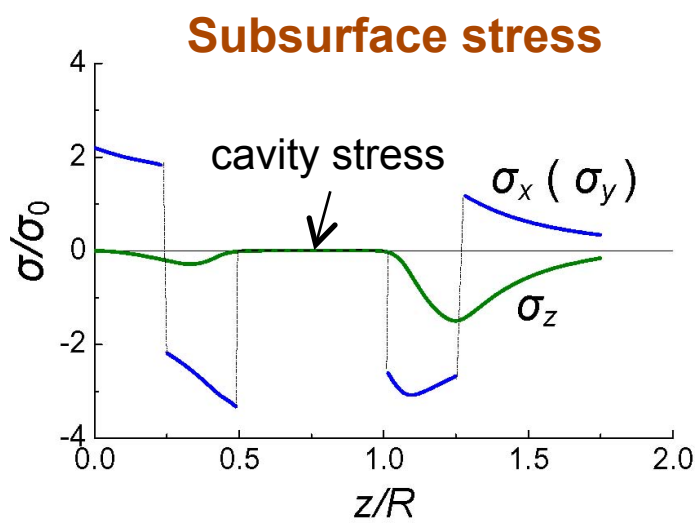


Near-surface inhomogeneous inclusion (depth *h*) subject to dilatation eigenstrain

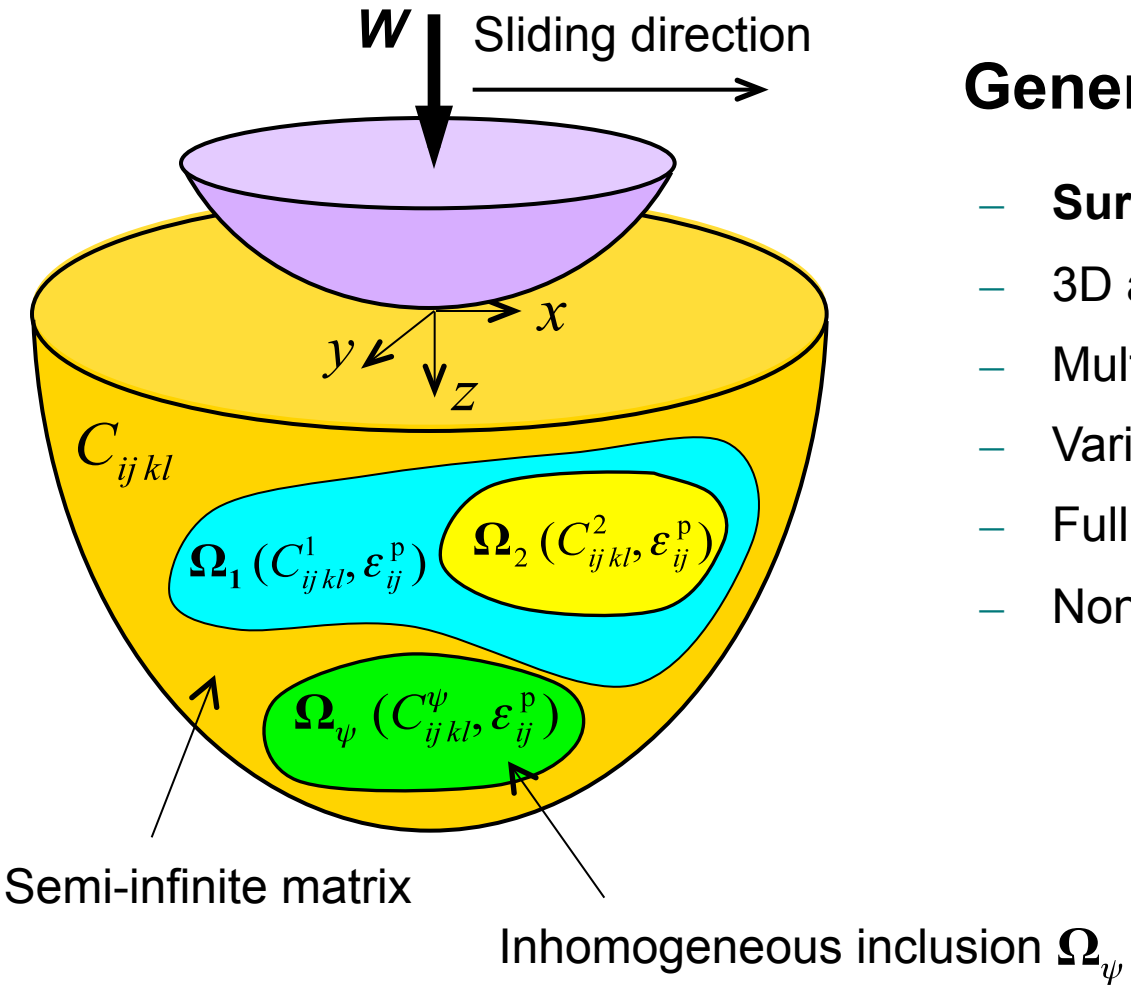
$$e_{ij} = \alpha T \delta_{ij}$$

Normalization stress: $\sigma_o = E\alpha T / 3(1-\nu)$





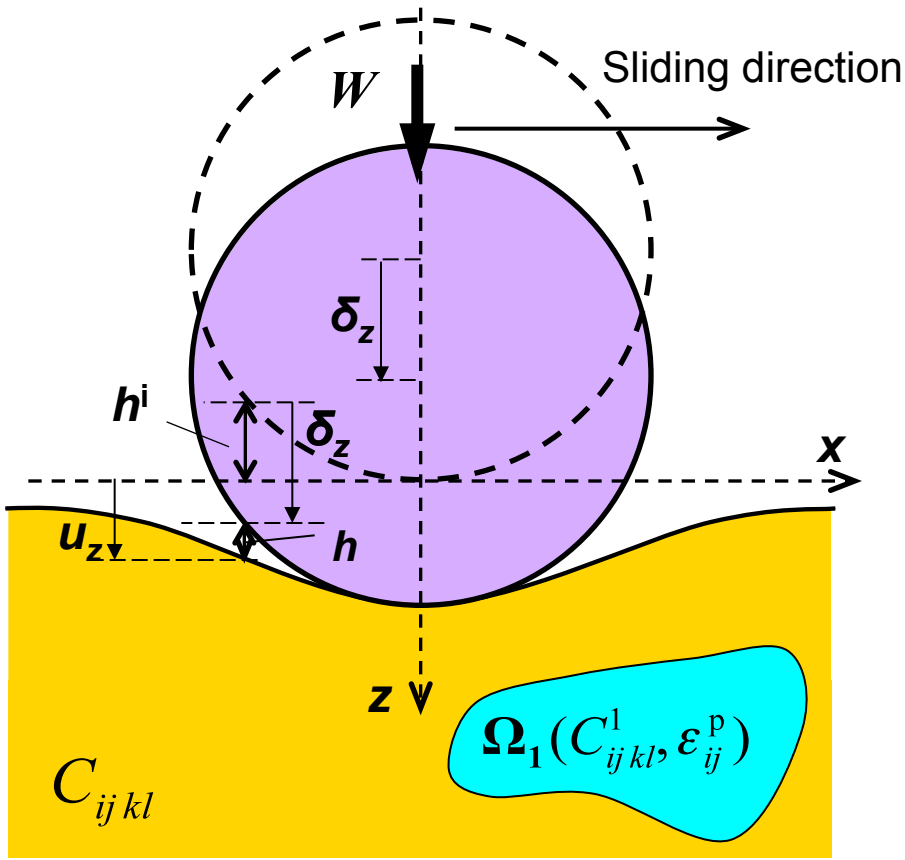
Inhomogeneous Inclusions Near Surfaces in Contact



Generality

- **Surface contact loading**
- 3D arbitrary shape
- Multiple number
- Various materials
- Full interactions
- Non-uniform initial eigenstrain ε^p_{ij}

Description of Contacting Surfaces



Force balance

$$W = \iint_{A_c} p(x,y)\,\mathrm{d}x\mathrm{d}y$$

Surface gap equations

$$h(x,y) = h^{\mathrm{i}}(x,y) + u_z(x,y) - \delta \geq 0$$

$$p(x,y) > 0, \quad h(x,y) = 0, \qquad (x,y) \in A_c$$

$$p(x,y) = 0, \quad h(x,y) > 0, \qquad (x,y) \notin A_c$$

Boundary conditions ($z = 0$)

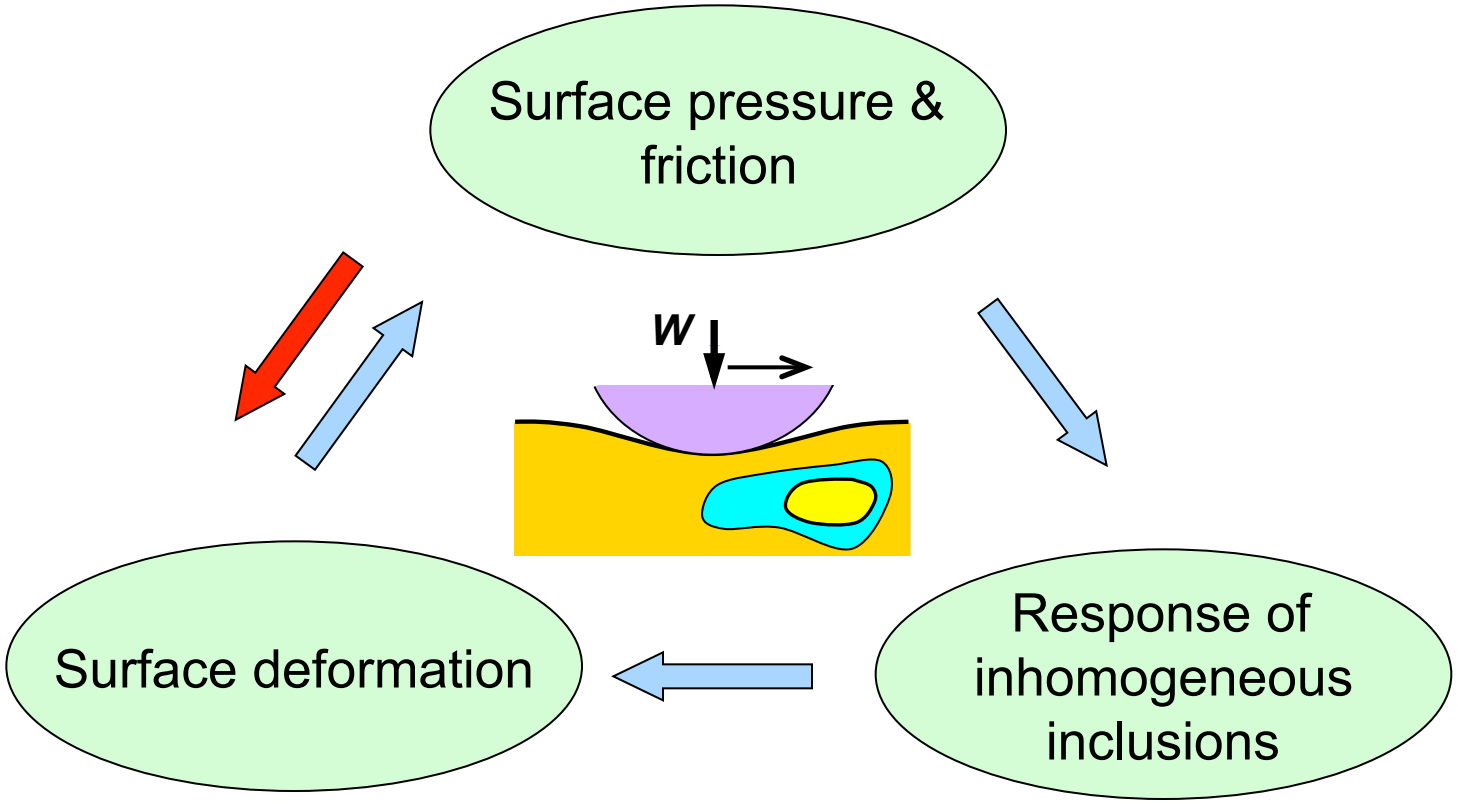
$$\sigma_{zz} = -p$$

$$\sigma_{xz} = -q \qquad (q = \mu p)$$

$$\sigma_{yz} = 0$$

Unknown contact area and contact pressure to be determined

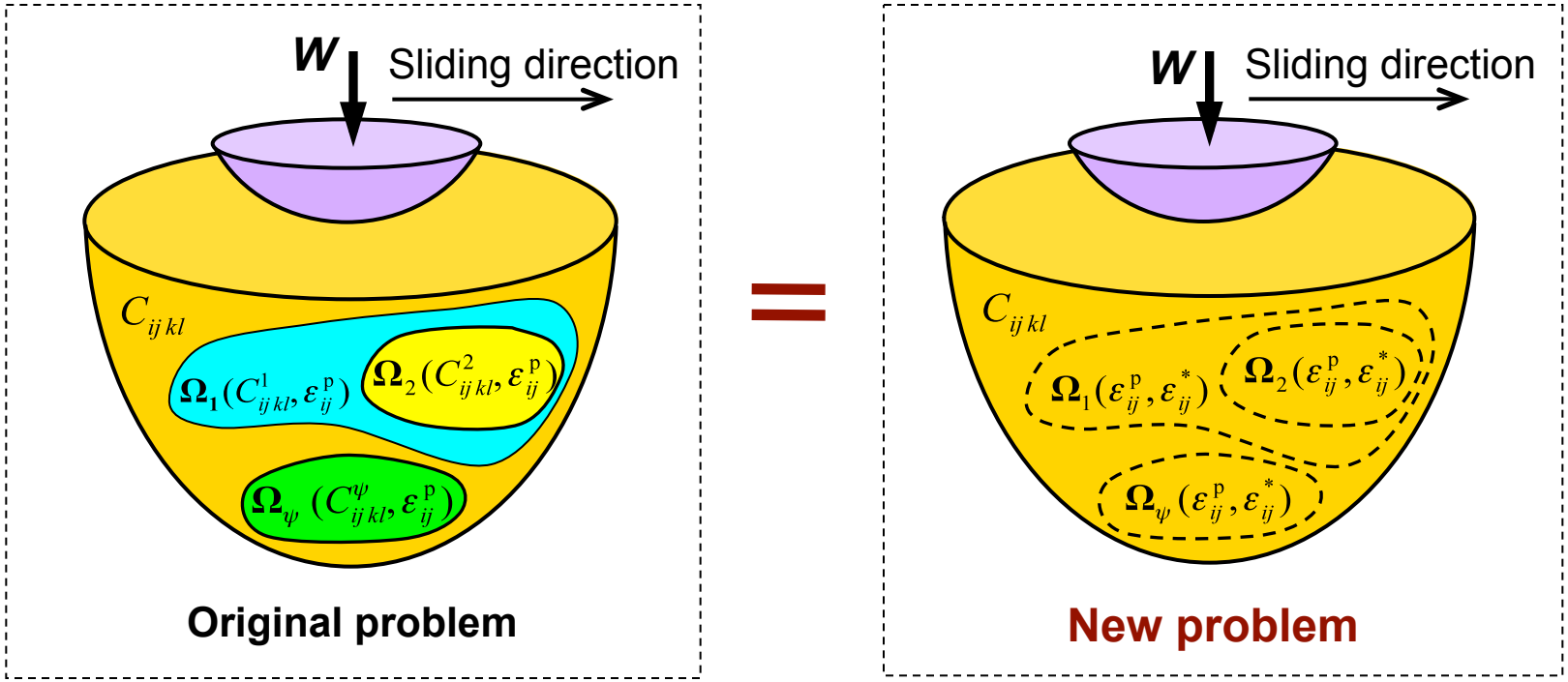
Interactions Between Loading Body and Inhomogeneous Inclusions



Surface displacement is due to:

1) surface pressure and friction, and 2) inhomogeneous inclusions.

Equivalent Inclusion Method

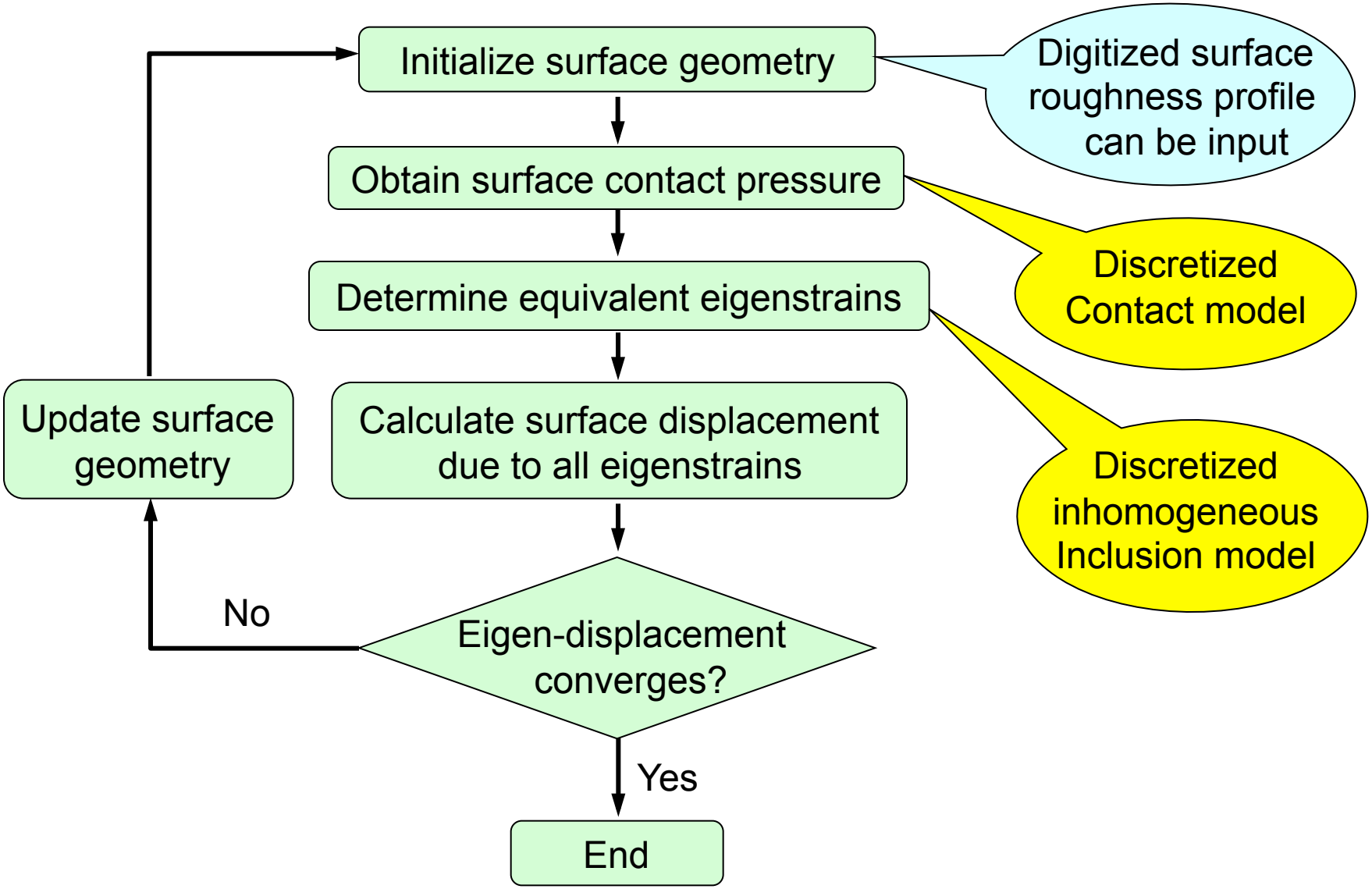


New problem is decomposed into two interacting sub-problems:

1. Homogenous inclusions problem (unknown equivalent eigenstrains ε^*_{ij})

2. Homogeneous half-space contact problem (unknown contact pressure)

Algorithm to Integrate Two Sub-Problems



Elastic-Plastic Indentation Model

An elastic-plastic indentation model is further developed based on the inhomogeneous inclusion solution by incorporating:

- **von Mises yield criterion**

$$f = \sigma_{\mathrm{vm}} - \sigma_{\mathrm{y}} = \sqrt{\frac{3}{2} S_{ij} S_{ij}} - \sigma_Y > 0 \qquad S_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij}$$

- **Flow rule (Hill, 1950)**

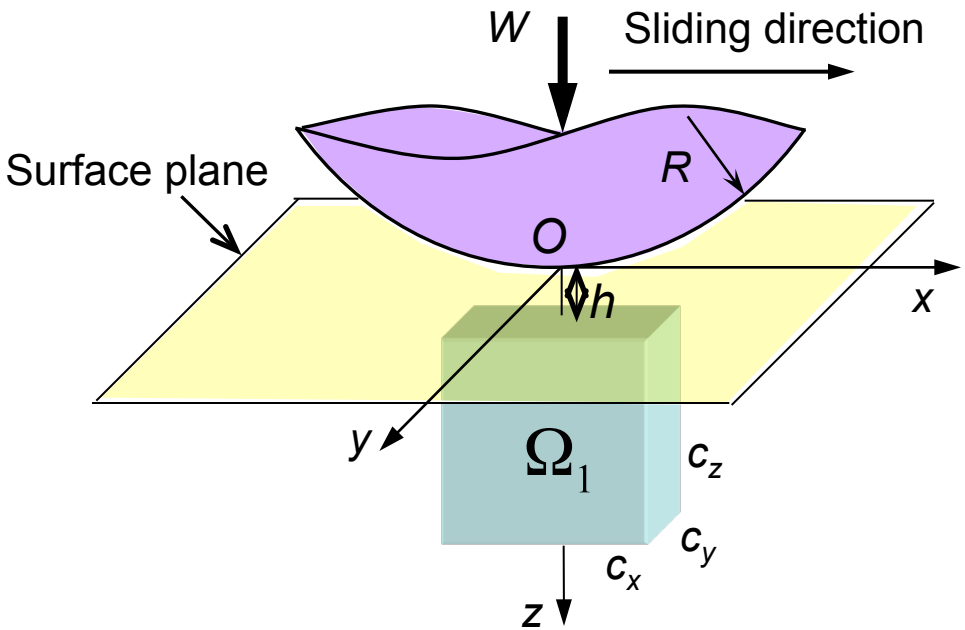
$$\mathrm{d}\varepsilon_{ij}^{\mathrm{p}} = \mathrm{d}\lambda \frac{\partial f}{\partial \sigma_{ij}} = \mathrm{d}\lambda \frac{\partial S_{ij}}{\partial \sigma_{\mathrm{vm}}} \qquad \lambda = \sum \sqrt{2\mathrm{d}\varepsilon_{ij}^{\mathrm{p}} \mathrm{d}\varepsilon_{ij}^{\mathrm{p}} / 3}$$

$\mathrm{d}\lambda$: equivalent plastic strain increment

- **Incremental load process (iterative algorithm)**

Contents

A Single Inhomogeneous Inclusion



Materials parameters

Indenter: rigid

Matrix: E_m = 210 GPa, v_m = 0.28

Inclusion: $E_i = Y E_m$, v_i = 0.28

Dimensions of Ω_1

Size: $c_x = c_y = c_z = 2a_0/3$

Depth: $h = a_0/3$

Solution for a homogenous half-space under frictionless spherical indentation (Hertz, 1882):

Contact radius: $a_0 = \left(\dfrac{3WR}{4E^*}\right)^{1/3}$

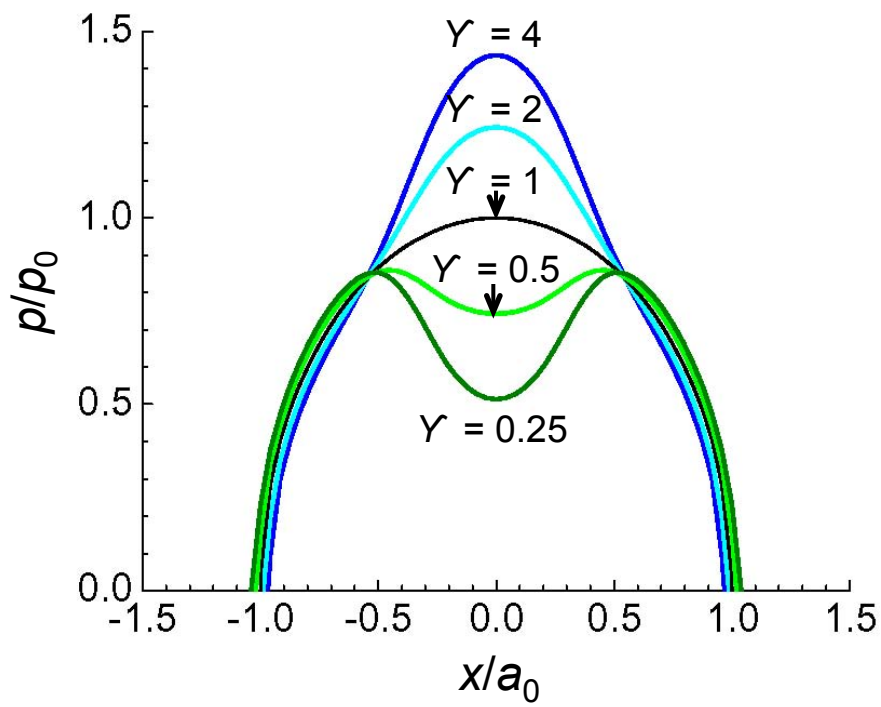
Maximum contact pressure: $p_0 = \dfrac{3W}{2\pi a_0^2}$

Material Effect

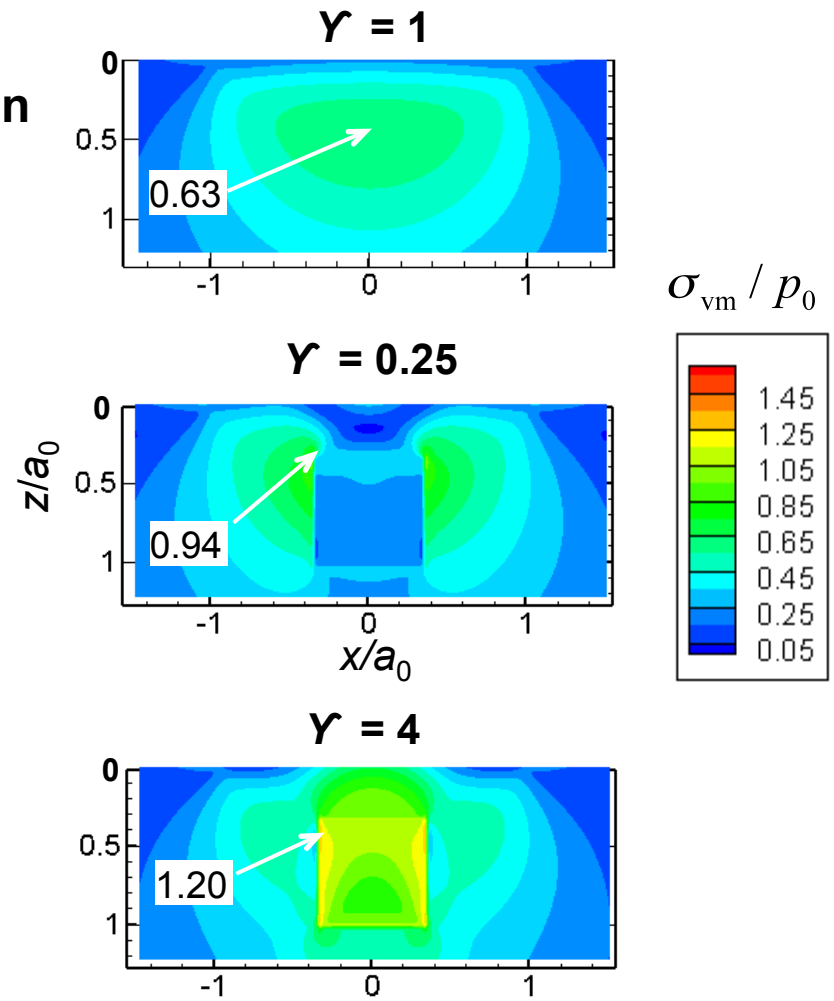
Υ > 1: stiff inhomogeneous inclusion

Υ < 1: compliant inhomogeneous inclusion

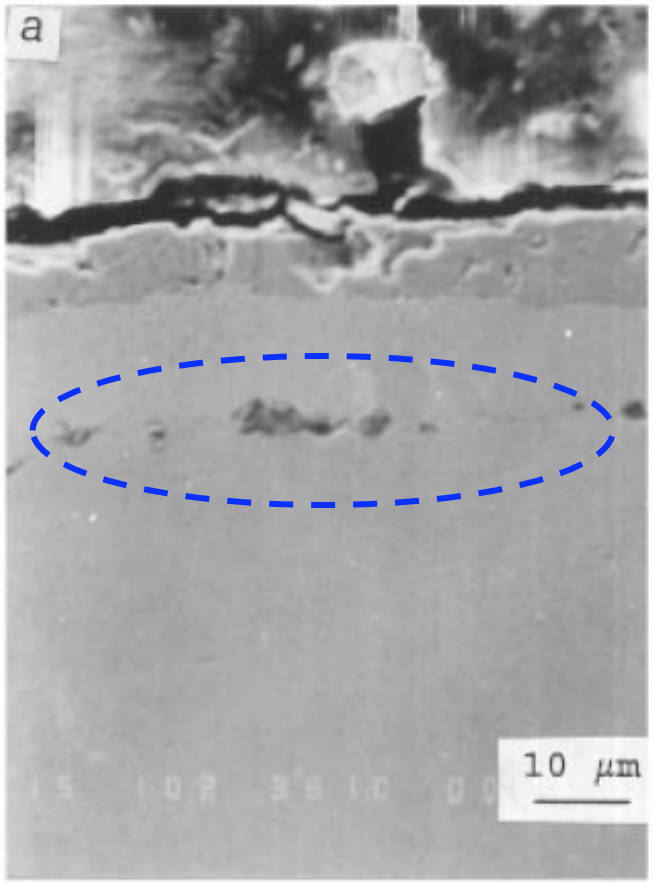
Frictionless surface ($\mu = 0$)



Normal surface pressure

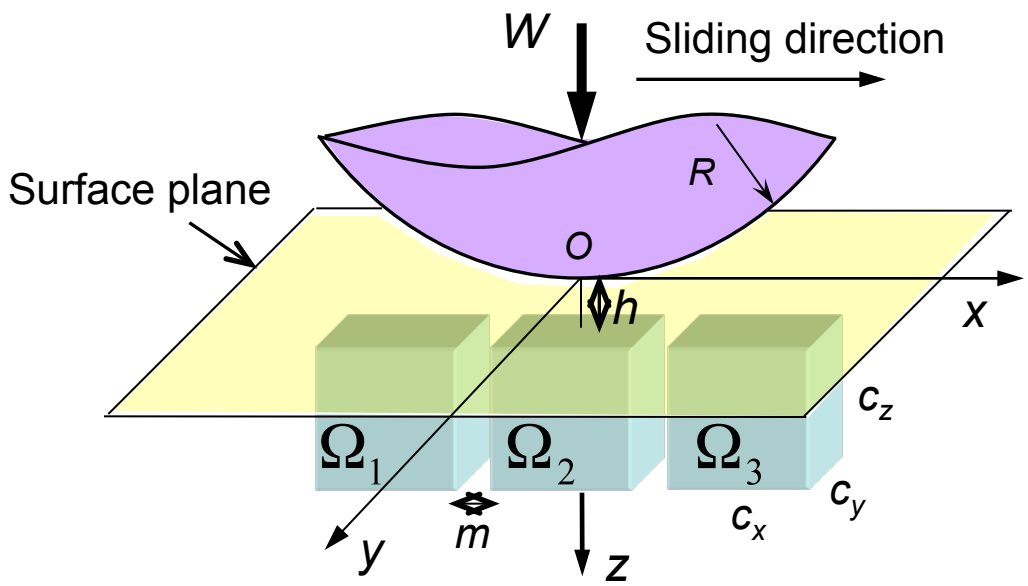


Subsurface von Mises stresses in the central plane $y = 0$



A stringer of aluminum oxides (Al_2O_3) in steel (Ray *et al.*, 1999)

A Stringer of Inhomogeneous Inclusions



Material parameters

Indenter: rigid

Matrix (steel): E_m = 210 GPa, v_m = 0.28

Inhomogeneous Inclusion (Al_2O_3): E_i = 344 GPa, v_i = 0.25

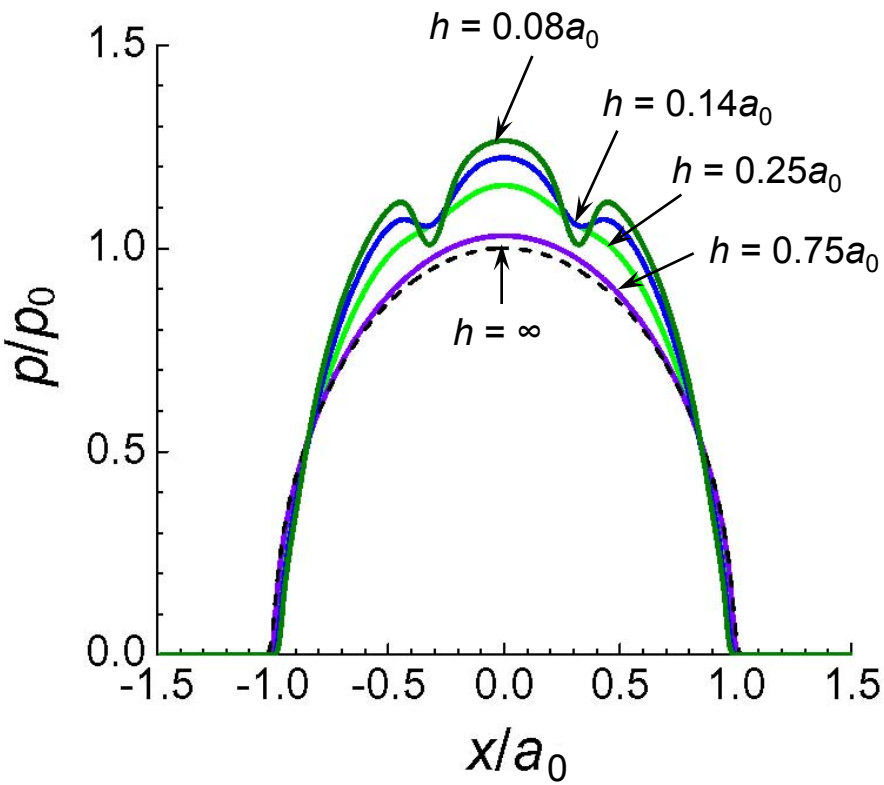
Dimensions of Ω_i

Size: $c_x = c_y = c_z = 0.5\ a_0$

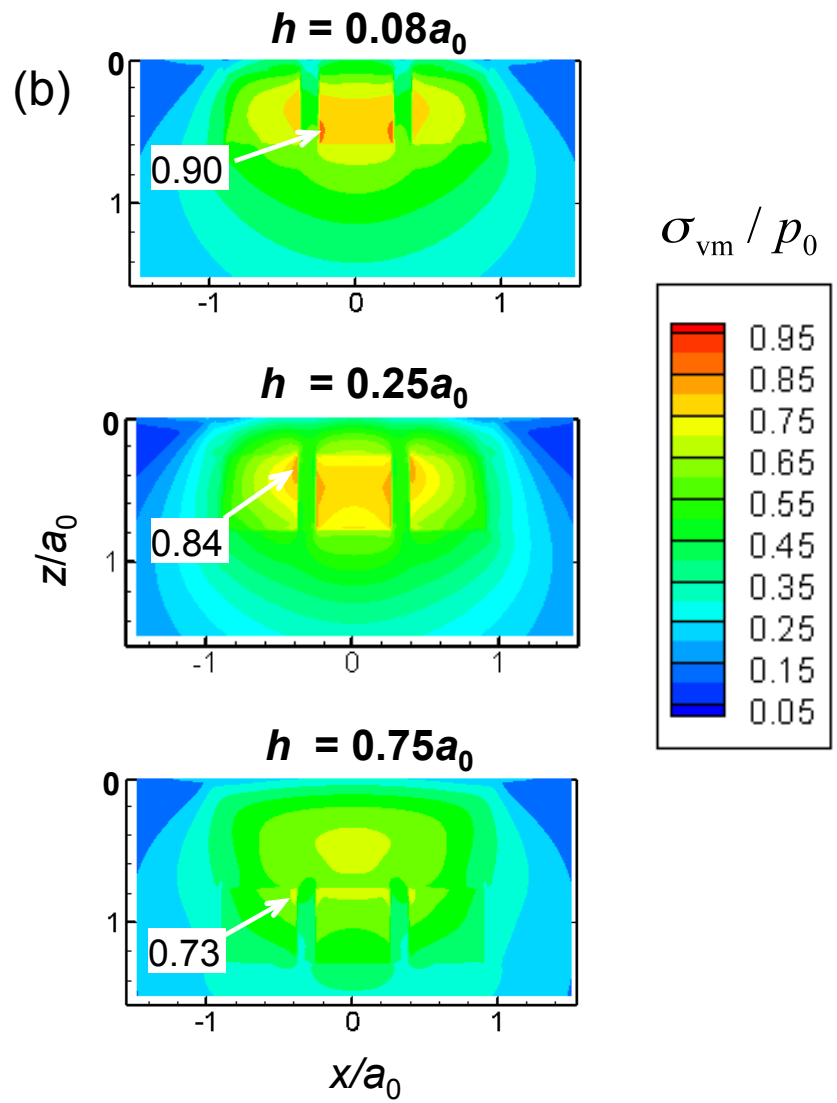
Spacing: $m = 0.125\ a_0$

Depth Effect

Frictionless surface ($\mu = 0$)



Normal surface pressure

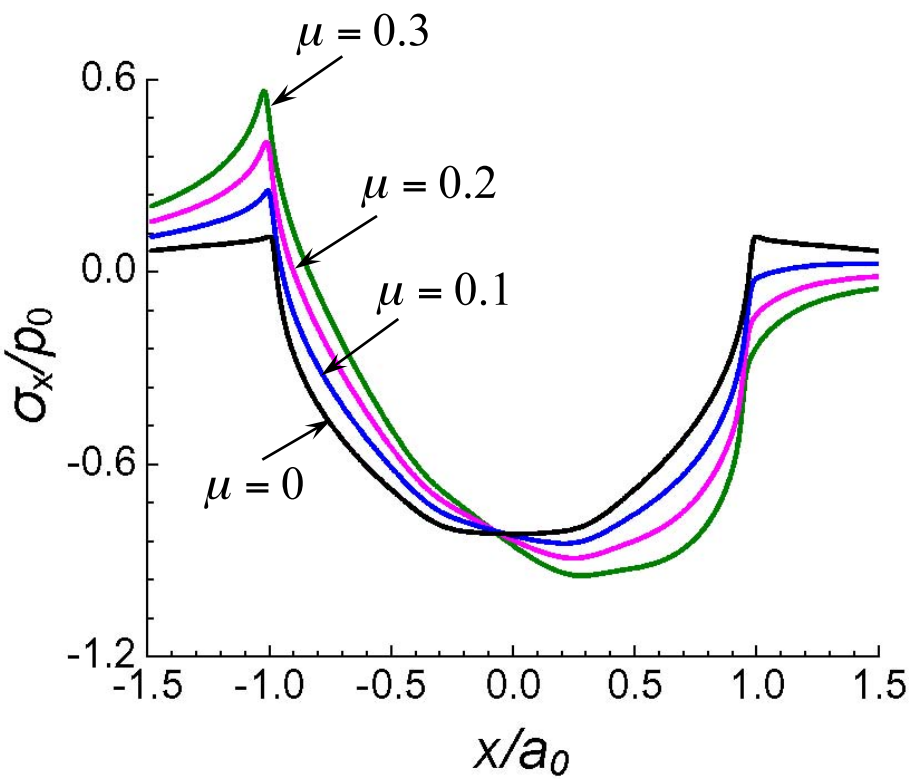


Subsurface von Mises stresses in the central plane $y = 0$

Friction Effect

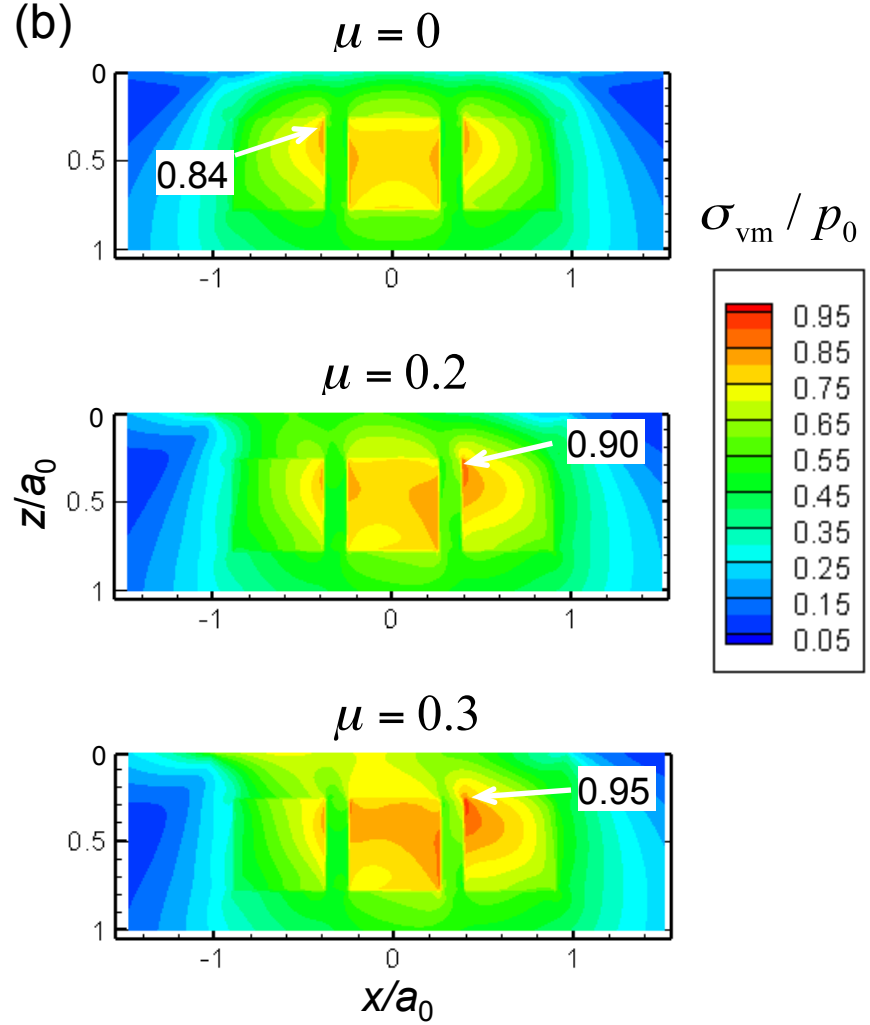
(a)

Depth $h = 0.25a_0$



Surface stress component σ_x

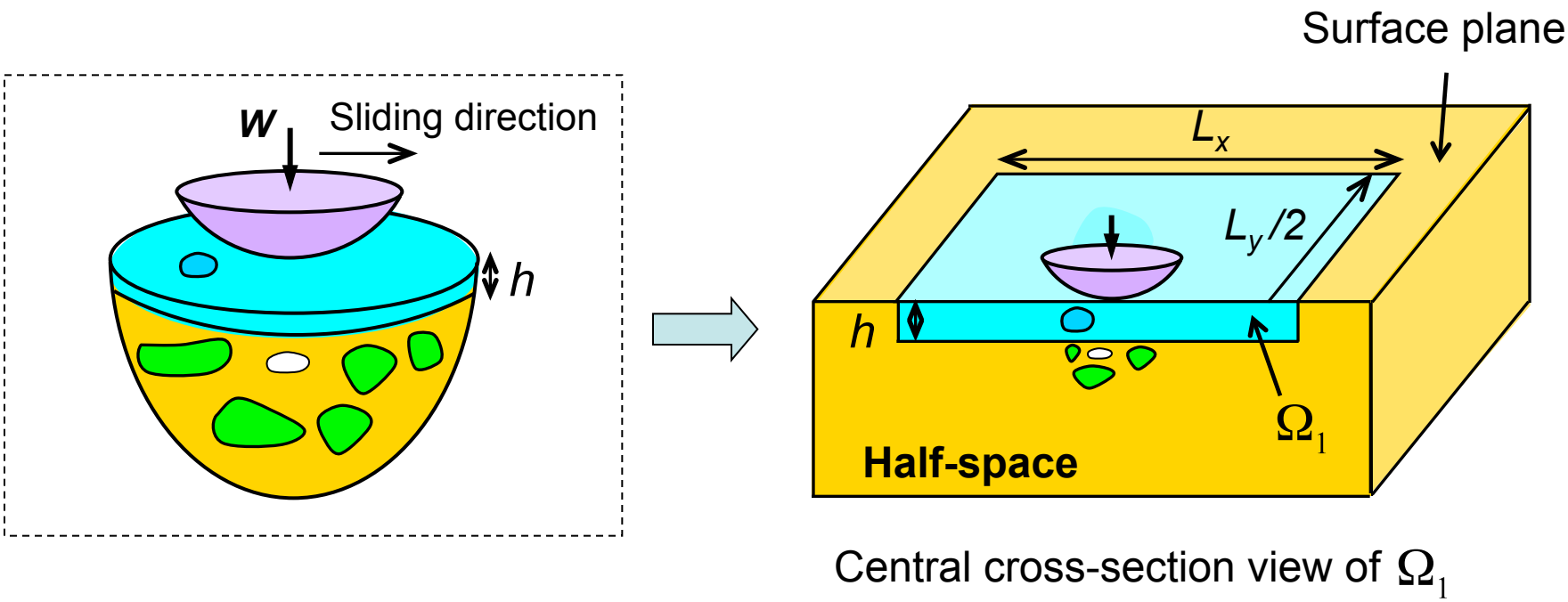
(b)



Sub-surface von Mises stresses

Novel Application: Film-Substrate Systems

A film of thickness *h* is modeled as an inhomogeneous inclusion Ω_1 of dimensions $L_x \times L_y \times h$ embedded in a half-space.



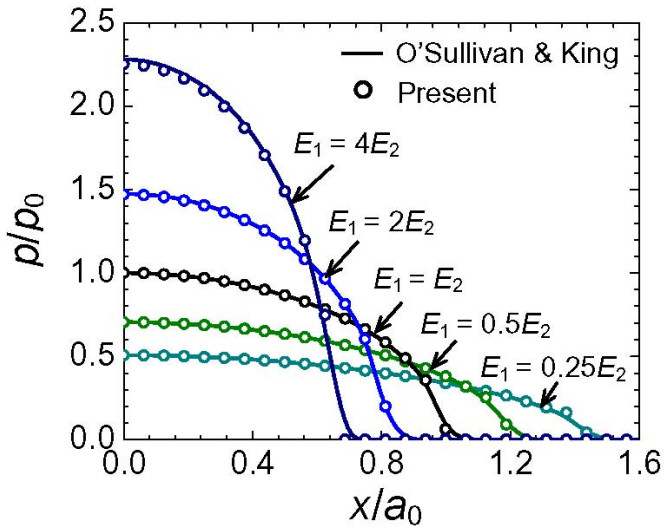
Modeling conditions:

- L_x, L_y >> h ; L_x, L_y >> contact area dimensions
- $\sigma_{ij} \approx 0$ at the vertical edge planes of Ω_1

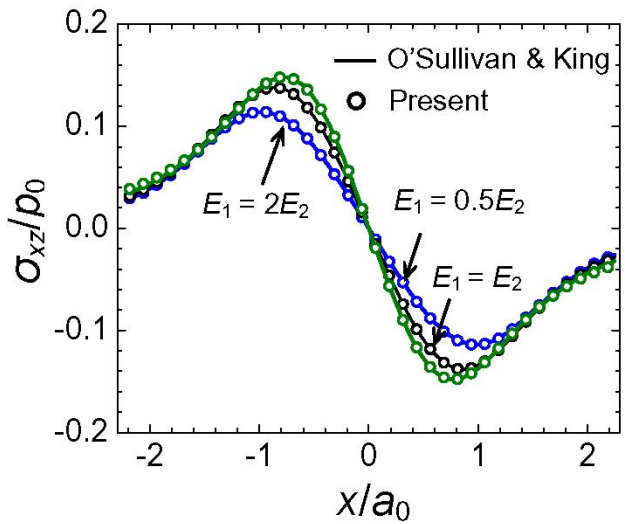
Model Validation

- Compared with an analytic solution for elastic indentation of thin films (O'Sullivan & King, 1988)

Film: E_1; Substrate: E_2; Film thickness: a_0



Normal surface pressure



σ_{xz} at the film/substrate interface

- Compared with experimental load-displacement curves for elastic-plastic indentation of DLC films on steel by a diamond indenter (Michler *et al.,* 1999)

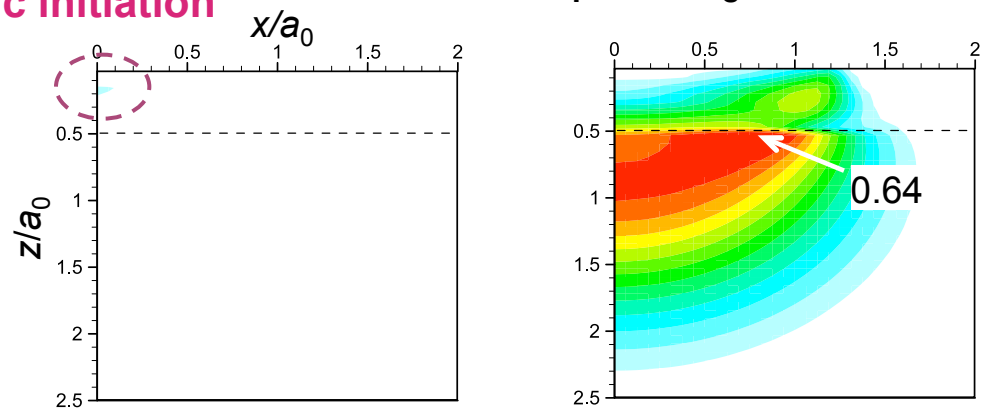
Elastic-Plastic Indentation on Coated Surfaces

W_c **:** critical indentation load to initiate plastic deformation in a homogenous half-space of E_s.

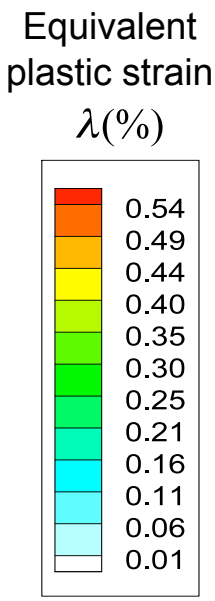
Both yield strengths of stiff and compliant films are 1.5 times that of the substrate.

Film thickness: $0.5a_0$

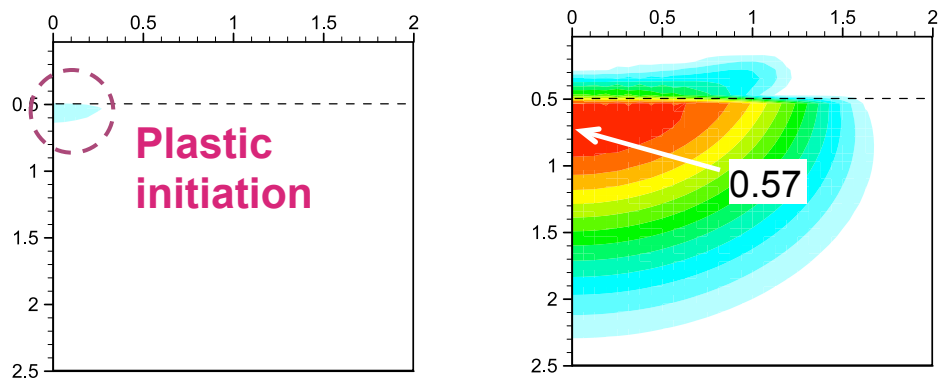
Stiff film (E_f = 2 E_s)



Load at $1.5W_c$ Final load at $30W_c$

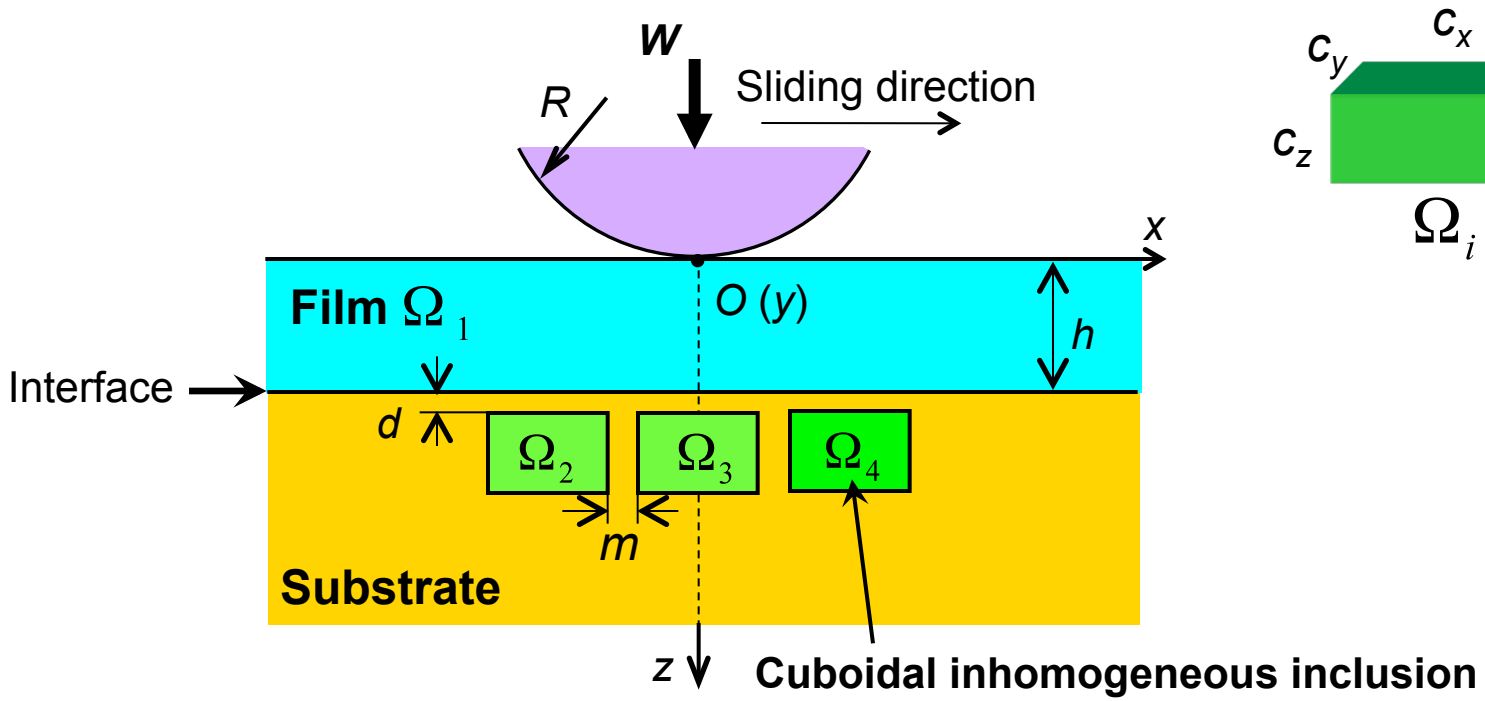


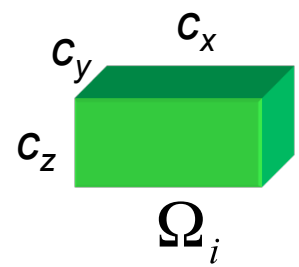
Compliant film (E_f = 0.25 E_s)



Load at $4.5W_c$ Final load at $30W_c$

A Stringer of Inhomogeneous Inclusions Beneath the Film-Substrate Interface





Indenter: rigid

Substrate (steel): E_s = 210 GPa, ν_s = 0.28

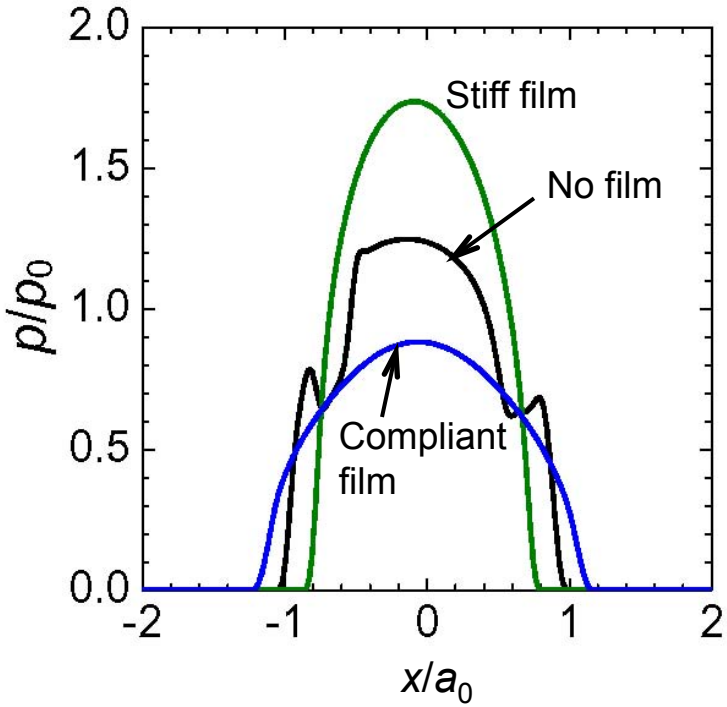
Inhomogeneous inclusion (Al_2O_3): E_i = 344 GPa, ν_i = 0.25

Friction coefficient: μ = 0.3

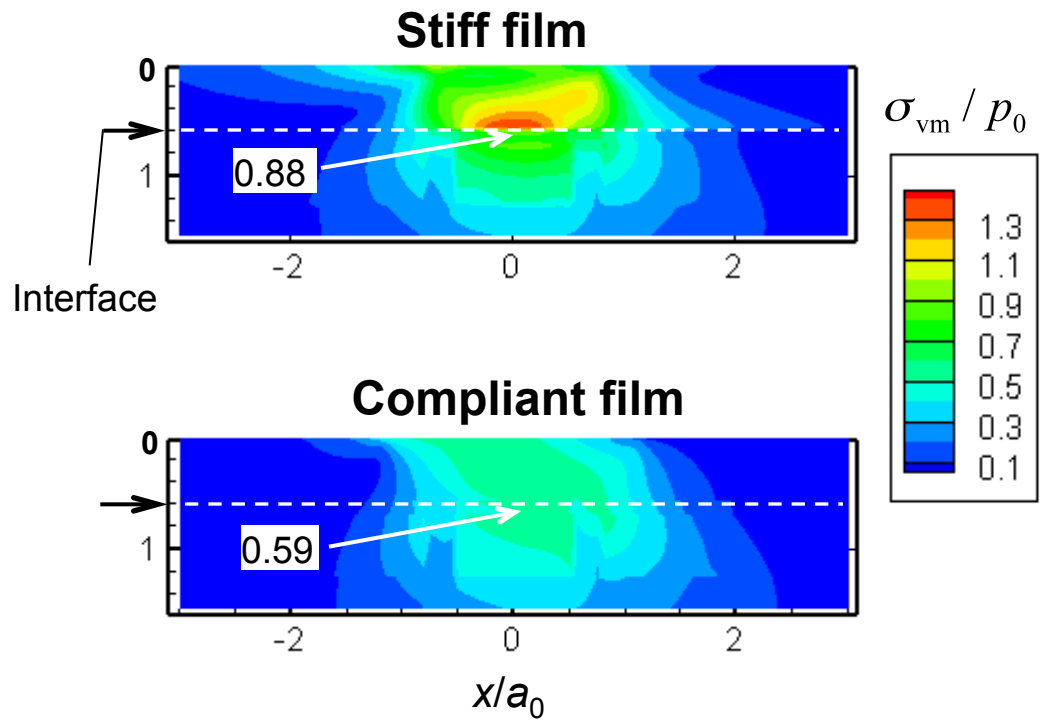
Size: $c_x = c_y = c_z = 0.5\ a_0$

Spacing: $m = 0.125\ a_0$

Comparison Between Stiff and Compliant Films



Normal surface pressure



Subsurface von Mises stresses

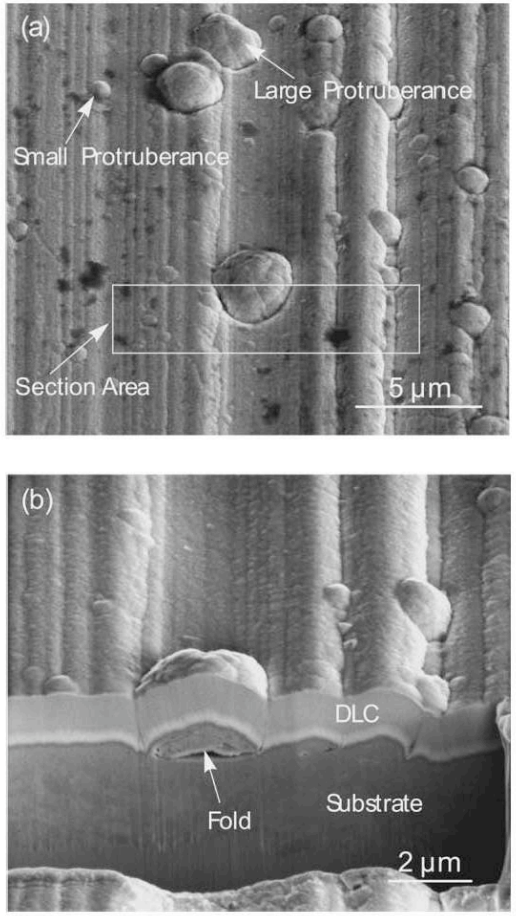
Substrate (Steel): E_s = 210 GPa

Stiff film (WC): E_f = 640 GPa

Compliant film (W-DLC): E_f = 110 GPa

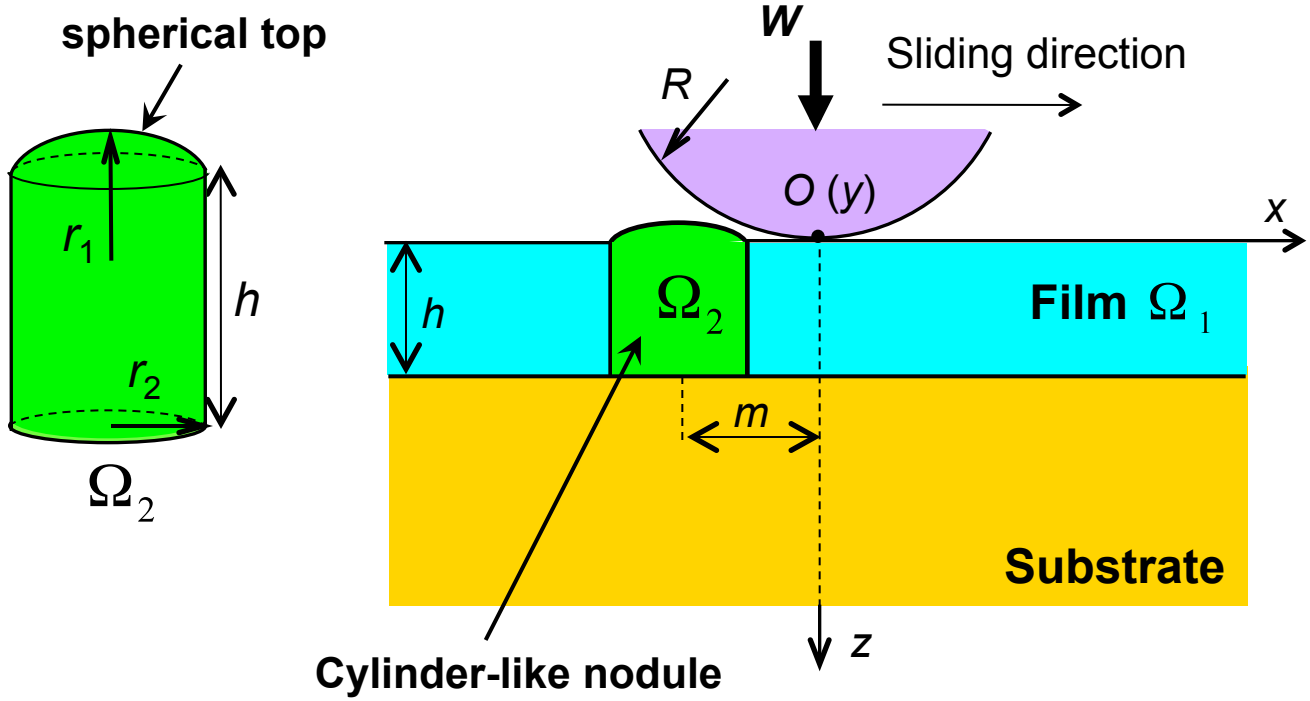
Film thickness: $h = 0.6\ a_0$

Friction coefficient: $\mu = 0.3$



Nodules in a DLC film on steel (Wang *et al.*, 2002)

A Nodule in the Film



Film thickness: $h = a_0$

Nodule: $r_1 = 3a_0$; $r_2 = 0.5a_0$

Indenter: rigid

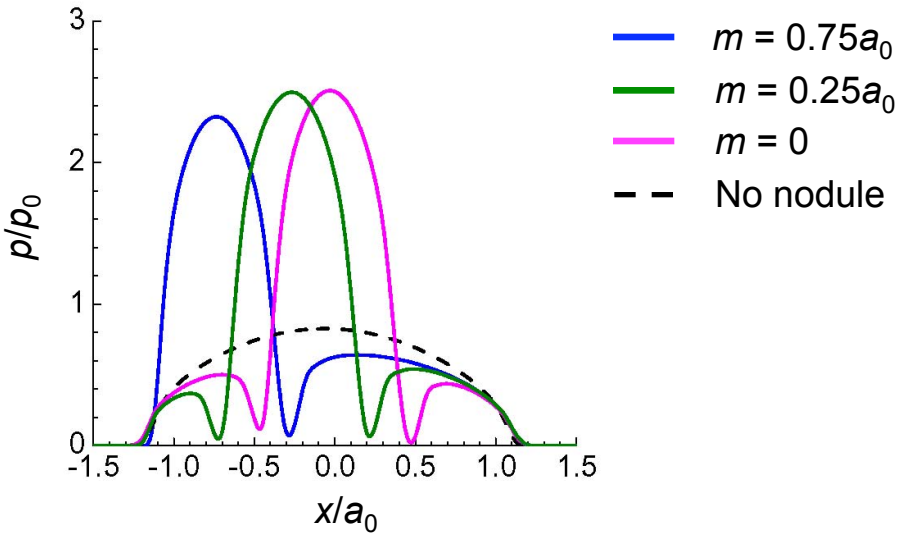
Substrate (steel): E_s = 210 GPa

Film (W-DLC) : E_f = 110 GPa

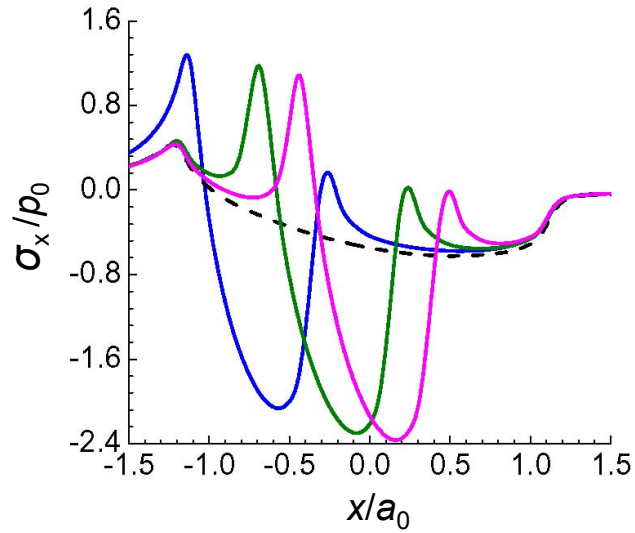
Nodule: E_n = 121 GPa

Friction coefficient: μ = 0.3

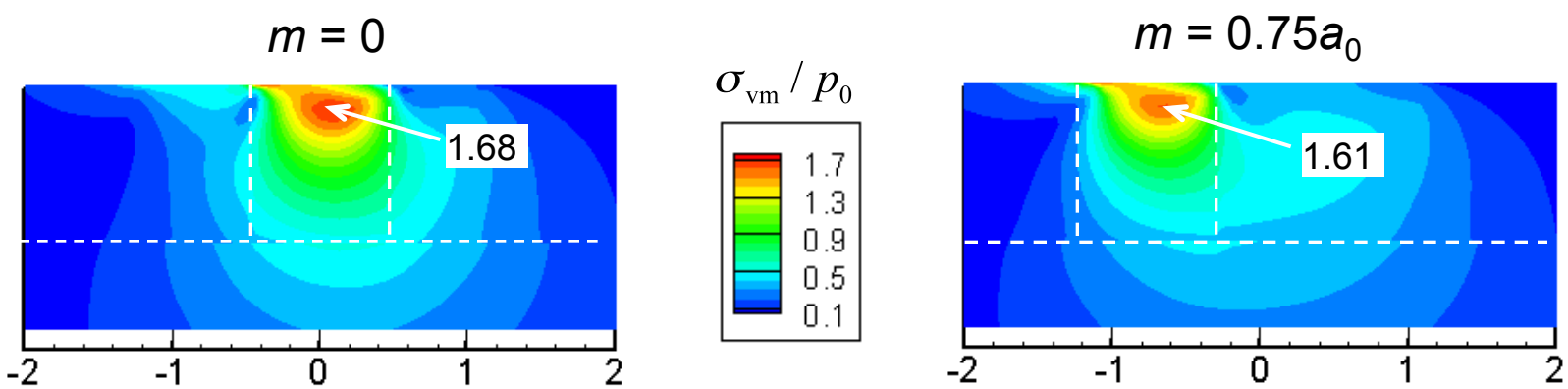
Nodule Location Effect



Normal surface pressure



Surface stress component σ_x

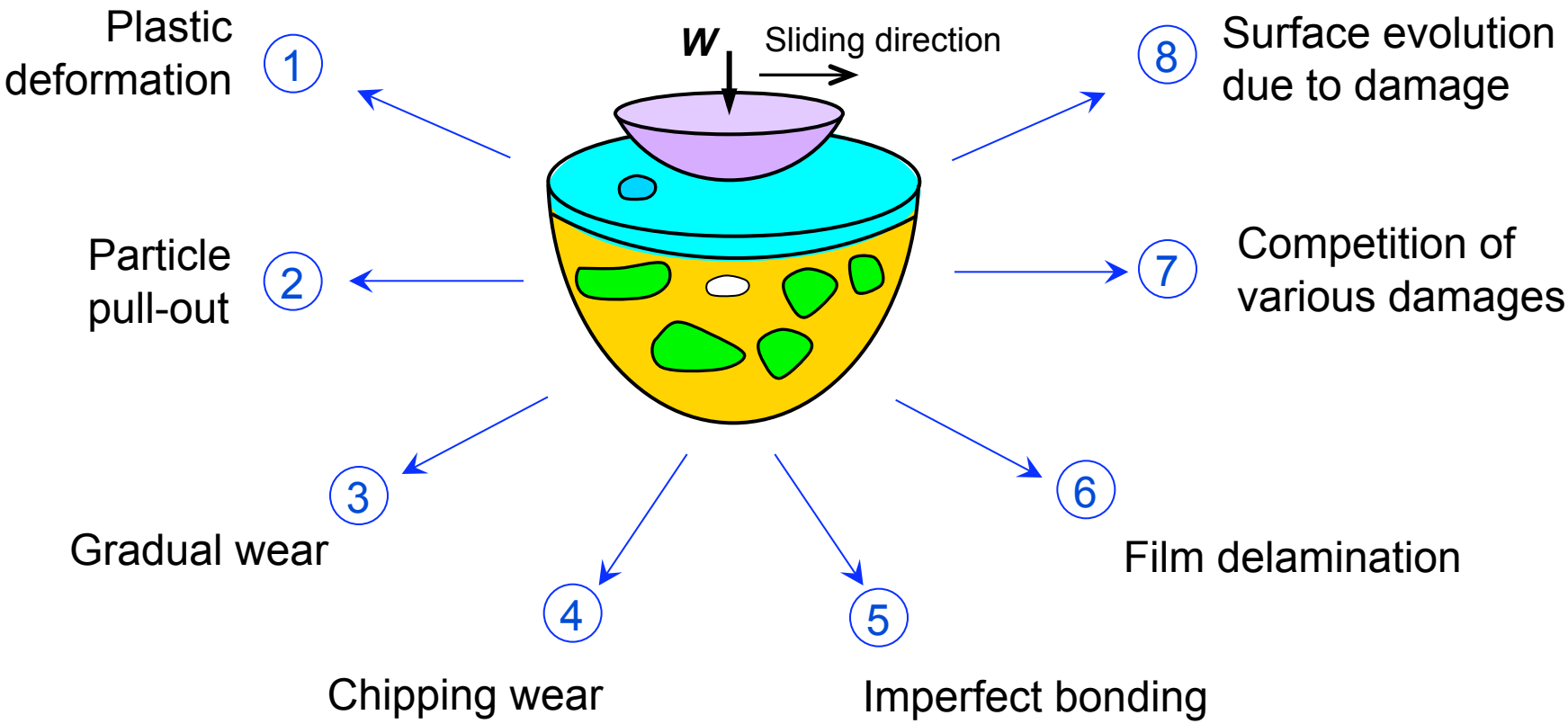


Subsurface von Mises stresses

Contents

Conclusions

- A unified theory was developed to model damage to real surfaces.



Conclusions

- This theory can address challenging surface engineering problems involving material dissimilarity and inelastic deformation.
- The solution of multiple inhomogeneous inclusions of 3D arbitrary shape near surfaces in contact was developed.
- The solution considers interactions between all the inhomogeneous inclusions and between them and the loading body.
- A layer of film was modeled as an inhomogeneous inclusion, leading to the successful modeling of film-substrate systems.

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Thank you!