A Unified Theory for Modeling Damage to Real Surfaces in Contact

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- Development of Theory
- Applications of Theory
- Conclusions
Applications of Surfaces in Contact

Aerospace

Biomedical

Energy

MEMS & NEMS

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

- Materials
- Operation Conditions
- Topographies
- Imperfections
- Surface & Subsurface
- Lubrication
- Surface Treatment

- Metal
- Ceramic
- Composite
- Gas
- Liquid
- Grease
- Solid
- Coating
- Carburizing

- Mechanical
- Thermal
- Electrical
- Macro
- Micro
- Nano
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

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 $\varepsilon^p$

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

Temperature raised by $\Delta T$ in a constrained 1D bar

Free thermal expansion

Mechanical deformation

Total strain: $\varepsilon = 0$

$\Delta l = \alpha \Delta T l$

$\varepsilon^p = \alpha \Delta T$

$\varepsilon^e = -\alpha \Delta T$

$\varepsilon = \varepsilon^p + \varepsilon^e = 0$

Stress: $\sigma = E \varepsilon^e = -E \alpha \Delta T$ (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.

1. Plastic deformation
2. Particle pull-out
3. Gradual wear
4. Chipping wear
5. Imperfect bonding
6. Film delamination
7. Competition of various damages
8. Surface evolution due to damage

Sliding direction

W
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

Infinite space

Loaded surfaces

Surfaces in contact

I. Infinite space

II. Loaded surfaces

Coated surfaces in contact

Sliding direction

$\sigma^\infty$

$p(x, y)$

$q(x, y)$

$w$

$w$

Coating

Surfaces in contact
Inhomogeneous Inclusions Near Surfaces

Generality

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

Semi-infinite matrix

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

**Hooke’s law:**

\[ \sigma_{ij} = C_{ijkl}^p(\varepsilon_{kl} - \varepsilon_{kl}^p) \quad (1) \]

**Decomposition:**

\[ \sigma_{ij} = C_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^p - \varepsilon_{kl}^*) \quad (2) \]

**Unknown equivalent eigenstrains $\varepsilon_{ij}^*$ depend on:**

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

**Eqs.(1)-(3)**
Eq. (4) is not solvable until we determine:

- Eigenstress-eigenstrain relationship (solution for homogenous inclusions)
  \[ \sigma^* \text{ is expressed in terms of } \varepsilon^* \quad ; \quad \sigma^p \text{ is expressed in terms of } \varepsilon^p \]

- Stresses due to normal and tangential tractions at the surface
  \[ \sigma^0 \leftarrow p(x, y) \text{ and } q(x, y) \]
Eigenstress-Eigenstrain Relationship
(Solution for Homogeneous Inclusions $\Omega_\psi$)

Discretization method: each $\Omega_\psi$ is approximated by many small cuboids.

- **Uniform eigenstrain in each cuboid**
- **Non-uniform eigenstrain in each $\Omega_\psi$**

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

$$\sigma^\psi_{\alpha\beta\tau} = \sum_{\mu=0}^{N_x-1} \sum_{\nu=0}^{N_y-1} \sum_{\lambda=0}^{N_z-1} A_{\alpha-\mu,\beta-\nu,\tau-\lambda} z^\mu_l z^\nu_l z^\lambda_l$$ (5)

$$\sigma^\psi_{\alpha\beta\tau} = \sum_{\mu=0}^{N_x-1} \sum_{\nu=0}^{N_y-1} \sum_{\lambda=0}^{N_z-1} A_{\alpha-\mu,\beta-\nu,\tau-\lambda} z^\mu_l z^\nu_l z^\lambda_l$$ (6)

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

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

Half-space surface

Cuboidal void

Near-surface inhomogeneous inclusion (depth $h$) subject to dilatation eigenstrain $e_{ij} = \alpha T \delta_{ij}$

Normalization stress: $\sigma_o = E\alpha T / (1 - \nu)$
Inhomogeneous Inclusions Near Surfaces in Contact

- Surface contact loading
- 3D arbitrary shape
- Multiple number
- Various materials
- Full interactions
- Non-uniform initial eigenstrain $\varepsilon_{ij}^p$
Description of Contacting Surfaces

Force balance

\[ W = \int \int_{A_c} p(x, y) \, dx \, dy \]

Surface gap equations

\[ h(x, y) = h^i(x, y) + u_z(x, y) - \delta \geq 0 \]
\[ p(x, y) > 0, \quad h(x, y) = 0, \quad (x, y) \in A_c \]
\[ p(x, y) = 0, \quad h(x, y) > 0, \quad (x, y) \notin A_c \]

Boundary conditions (z = 0)

\[ \sigma_{zz} = -p \]
\[ \sigma_{xz} = -q \quad (q = \mu p) \]
\[ \sigma_{yz} = 0 \]

Unknown contact area and contact pressure to be determined
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 $\varepsilon_{ij}^*$)
2. Homogeneous half-space contact problem (unknown contact pressure)
Algorithm to Integrate Two Sub-Problems

1. Initialize surface geometry
2. Obtain surface contact pressure
3. Determine equivalent eigenstrains
4. Calculate surface displacement due to all eigenstrains
5. Update surface geometry
6. Check if eigen-displacement converges?
   - Yes: End
   - No: Go back to Initialize surface geometry

- Digitized surface roughness profile can be input
- Discretized Contact model
- Discretized inhomogeneous Inclusion model
Elastic-Plastic Indentation Model

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

- **von Mises yield criterion**

  \[ f = \sigma_{vm} - \sigma_y = \sqrt{\frac{3}{2}} S_{ij} S_{ij} - \sigma_y > 0 \]

  \[ S_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij} \]

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

  \[ d\varepsilon_{ij}^p = d\lambda \frac{\partial f}{\partial \sigma_{ij}} = d\lambda \frac{\partial S_{ij}}{\partial \sigma_{vm}} \]

  \[ \lambda = \sum \sqrt{2 d\varepsilon_{ij}^p d\varepsilon_{ij}^p / 3} \]

  \( d\lambda \): equivalent plastic strain increment

- **Incremental load process (iterative algorithm)**
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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 $\Omega_1$

- 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: $a_0 = \left( \frac{3WR}{4E^*} \right)^{1/3}$

Maximum contact pressure:

$p_0 = \frac{3W}{2 \pi a_0^2}$
Material Effect

$\Upsilon > 1$: stiff inhomogeneous inclusion
$\Upsilon < 1$: 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 ($\text{Al}_2\text{O}_3$) in steel (Ray et al., 1999)
A Stringer of Inhomogeneous Inclusions

Material parameters

Indenter: rigid

Matrix (steel): $E_m = 210 \text{ GPa}$, $\nu_m = 0.28$

Inhomogeneous Inclusion (Al$_2$O$_3$): $E_i = 344 \text{ GPa}$, $\nu_i = 0.25$

Dimensions of $\Omega_i$

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 $\sigma_x$

(b) Sub-surface von Mises stresses

\[ \sigma_{vm} / p_0 \]

- $\mu = 0$
- $\mu = 0.2$
- $\mu = 0.3$

$\sigma_{vm}$

Legend:
- 0.95
- 0.85
- 0.75
- 0.65
- 0.55
- 0.45
- 0.35
- 0.25
- 0.15
- 0.05
Novel Application: Film-Substrate Systems

A film of thickness $h$ is modeled as an inhomogeneous inclusion $\Omega_1$ of dimensions $L_x \times L_y \times h$ embedded in a half-space.

Modeling conditions:

- $L_x, L_y \gg h$; $L_x, L_y \gg$ contact area dimensions
- $\sigma_{ij} \approx 0$ at the vertical edge planes of $\Omega_1$
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: $a_0$

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: $0.5a_0$
A Stringer of Inhomogeneous Inclusions Beneath the Film-Substrate Interface

Indenter: rigid
Substrate (steel): $E_s = 210$ GPa, $\nu_s = 0.28$
Inhomogeneous inclusion ($\text{Al}_2\text{O}_3$): $E_i = 344$ GPa, $\nu_i = 0.25$
Friction coefficient: $\mu = 0.3$

Size: $c_x = c_y = c_z = 0.5 a_0$
Spacing: $m = 0.125 a_0$
Comparison Between Stiff and Compliant Films

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: \( \mu = 0.3 \)
Nodule Location Effect

Normal surface pressure

Surface stress component $\sigma_x$

Subsurface von Mises stresses

$m = 0.75a_0$

$m = 0.25a_0$

$m = 0$

No nodule

$m = 0$

$m = 0.75a_0$

$m = 0.25a_0$

$m = 0$

No nodule

$m = 0$

$m = 0.75a_0$

$m = 0.25a_0$

$m = 0$

No nodule

$m = 0$

$m = 0.75a_0$

$m = 0.25a_0$

$m = 0$

No nodule
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Conclusions

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

- Plastic deformation
- Particle pull-out
- Gradual wear
- Chipping wear
- Imperfect bonding
- Film delamination
- Competition of various damages
- Surface evolution due to damage

Sliding direction

$W$
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!