Prediction and Multiscale Modeling of Corrosion and Wear

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Gun-bore erosion in artillery systems
Gun-bore erosion in artillery systems

Typical 360° magnifying borescope micrograph of LCCr/ 8 rpm/zone six charge-related second-quarter-life land and groove erosion near the bore origin (Sopoka, Rickarda and Dunn, Wear 258:2005, 659–670)
Gun-bore erosion in artillery systems

Typical magnifying borescope micrograph of HC-Cr/1 rph/zone six charge related midlife erosion at the 12:00 bore origin. (Sopoka, Rickarda and Dunn, Wear 258:2005, 659–670)

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Gun-bore erosion in artillery systems

 Typical SEM cross-sectional micrograph of HC-Cr/zone six charge related of land and groove substrate erosion through a micro-crack at the 12:00 bore origin (Sopoka, Rickarda and Dunn, *Wear* **258**:2005, 659–670)  

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Gun-bore erosion in artillery systems

Metallographic section of the electroplated Cr-on-steel 120 mm tube following 118 cannon firings (Underwood, Vigilante, Mulligan and Todaro, *ASME Trans.* 128:2006, 168–172)
Gun-bore erosion in artillery systems

Gun-bore erosion in artillery systems

- Gun-bore wear involves the simultaneous operation of three factors:
  - Thermal: heating, thermal gradient, thermal stress cracks, radiation, surface melting.
  - Chemical: reacting flow, gas-wall reactions, corrosion.
  - Mechanical: cracking, ablation, spallation.

- resulting in:
  - Micro and macro-pitting.
  - Condemnation.
The larger picture: Model-based certification

- Ultimate objective: **Certification** of complex systems by a rigorous quantification of design **margins** and performance **uncertainties**
- Performance of complex systems is difficult to quantify based on testing alone
- Model-based certification: Develop physics-based, high-fidelity models enabling rigorous quantification of performance uncertainties with a small number of tests
- System behavior often occurs on multiple length and time scales, requiring multiscale modeling
- Ultimate goal: Knob-free (first-principles) predictive simulation.
Wear – Multiscale modeling

Sopoka et al., Wear, 258, 659 (2005)
Yamaguchi et al., Science, 309, 393 (2005)

Mesoscale:
- plasticity
- diffusion
- fracture

Nanoscale:
- impurity absorption, mobility
- grain-boundary decohesion
- lattice defects, dislocations
- chemical reactions

Macroscale:
- wear rates
- life assessment
- certification

M1 Abrams Main Battle Tank
Model problem – Hydrogen embrittlement

- Possible mechanisms for step 3:
  - *Hydrogen-enhanced decohesion (HED)*
  - *Hydrogen-enhanced localized plasticity (HELP)*
  - *Hydrogen-related phase changes (HRPC)*
HE – Multiscale model

- Continuum diffusion, FE stress analysis
- Continuum plasticity, resolved plastic zone
- Renormalized cohesive law
- First-principles cohesive law

\[ X = H_2, H_2S, H^+ \ldots \]

Zoom of the CRACK TIP REGION

length

mm \hspace{1cm} \mu m \hspace{1cm} nm

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Cohesive laws – First principles

\[ t = \frac{\partial \phi}{\partial \delta} \]

Cohesive laws – – First principles


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Cohesive laws – First principles

• Ab initio cohesive laws:
  – Peak stress \(\sim\) theoretical strength
  – Critical opening displacement \(\sim\) atomic lattice spacing
  – Critical energy release rate \(\sim\) Relaxed surface energy
  – Cohesive length \(\sim\) atomic lattice spacing
  – Mesh resolution requirement \(\sim\) atomic lattice spacing

• Continuum stresses limited by yield stress, mesh size

• Cannot embed first-principles cohesive laws directly in continuum calculations

• Must upscale (coarse-grain, renormalize) the first-principles cohesive law to continuum scale
Cohesive laws – Upscaling

- Effective (upscaled) cohesive law:
  - $N$ interatomic planes, first-principles cohesive law
  - Rice-Beltz elastic correction
Cohesive law – Upscaling

*Ab-initio* cohesive law

\[
\phi(\delta)/2\gamma
\]

\[
\phi \sim \frac{C}{2}\delta^2
\]

\[
1 \leq \delta / \delta_c \leq 1
\]

Renormalized cohesive law

\[
\bar{\phi}(\bar{\delta})/2\bar{\gamma}
\]

\[
\bar{\phi} \sim \frac{\bar{C}}{2}\bar{\delta}^2
\]

\[
1 \leq \bar{\delta} / \bar{\delta}_c \leq 1
\]

Universal shape!

\[
\bar{\sigma}_c = \sigma_c / \sqrt{N}, \quad \bar{\delta}_c = \delta_c \sqrt{N}, \quad \bar{C} = C / N
\]

Metal, semiconductor, and ionic ceramic all fall on same universal curve

Cohesive laws – Upscaling

- Continuum cohesive law attains asymptotically a *universal asymptotic form* independent of the form of the atomistic cohesive law
- The renormalized peak stress scales as: $\sigma_c / \sqrt{N}$
- The renormalized COD scales as: $\delta_c \sqrt{N}$
- Surface energy is preserved under renormalization
- The only information from the atomistic cohesive law that passes to the continuum is: i) Initial slope; ii) Surface energy
- The renormalized cohesive zone size is automatically resolved by mesh size
HE – Multiscale model

Continuum diffusion, FE stress analysis

Continuum plasticity, resolved plastic zone

Renormalized cohesive law

First-principles cohesive law

$X = H_2, H_2S, H^+ \ldots$

Zoom of the CRACK TIP REGION

length

mm

μm

nm

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Segregation-enhanced decohesion

The Born-Haber cycle

\[ 2\gamma(\theta) = -\Delta H_s + 2\gamma(0) + E_{ad} \]


<table>
<thead>
<tr>
<th>$\Theta_H$ (ML)</th>
<th>$-\Delta H_s$ (J/m²)</th>
<th>$2\gamma(0)$ (J/m²)</th>
<th>$E_{ad}$ (J/m²)</th>
<th>$2\gamma(\theta)$ (J/m²)</th>
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</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>4.856</td>
<td>0</td>
<td>4.856</td>
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<td>0.25</td>
<td>-0.427</td>
<td>4.856</td>
<td>-0.748</td>
<td>3.681</td>
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<tr>
<td>0.50</td>
<td>-0.854</td>
<td>4.856</td>
<td>-1.516</td>
<td>2.486</td>
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<tr>
<td>1.00</td>
<td>-1.708</td>
<td>4.856</td>
<td>-2.550</td>
<td>0.598</td>
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</table>
Hydrogen-enhanced decohesion of Fe(110)

\[ \gamma(\theta) = \gamma(0)(1 - 1.0467\theta + 0.1687\theta^2) \]

First-principles calculations of coverage dependence of surface energy in Fe(110) (Jarvis, Hayes and Carter, Chem. Phys. Chem., 1, 55, 2001)
Cohesive law – Effect of H coverage

\[ \theta = \frac{\Gamma}{\Gamma_s} \]

Coverage vs. cohesive strength

\[ \tau(\delta, \theta) = \tau_c(\theta)(1 - \delta/\delta_c) \]
\[ \tau_c(\theta) = \tau_c(0)(1 - 1.0467\theta + 0.1687\theta^2) \]

Coverage vs. cohesive law
HE – Hydrogen diffusion

- Diffusion equation: \( C_t = \text{div}(MC \text{grad} \mu) = 0 \)
- Chemical potential: \( \mu = \mu_0(T) + RT \log(C/C_0) - pV \)
- Surface coverage: \( \Gamma = \Gamma^s/[1 + C^{-1} \exp(\Delta g/RT)] \)  
  (Langmuir-McLean)
- Boundary conditions:

\[
\begin{align*}
\mu &= \mu_{\text{env}} \\
J_n &= L(\delta)(\mu - \mu_{\text{env}}) \\
J_n &= 0
\end{align*}
\]
Hydrogen absorption paths and energies into Fe(100) and Fe(110)


$E_a = 1.0 \text{ eV}$

$E_a = 0.34 \text{ eV}$
Hydrogen diffusion in strained Fe

\[ D(T) = D_0 \exp\left(-\frac{\Delta E + \Delta ZPE}{k_B T}\right) \]

Hops between T-sites:

Volumetric deformation:

\[
F = \begin{bmatrix}
1 + \epsilon & 0 & 0 \\
0 & 1 + \epsilon & 0 \\
0 & 0 & 1 + \epsilon
\end{bmatrix}
\]

<table>
<thead>
<tr>
<th>ε (%)</th>
<th>( D_0 ) (10^{-7} \text{ m}^2/\text{s})</th>
<th>( \Delta E ) (eV)</th>
<th>( \Delta E + \Delta ZPE ) (eV)</th>
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</thead>
<tbody>
<tr>
<td>-2</td>
<td>1.872</td>
<td>0.095</td>
<td>0.044</td>
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<td>-1</td>
<td>1.814</td>
<td>0.094</td>
<td>0.046</td>
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<tr>
<td>0</td>
<td>1.818</td>
<td>0.092</td>
<td>0.044</td>
</tr>
<tr>
<td>1</td>
<td>1.730</td>
<td>0.092</td>
<td>0.048</td>
</tr>
<tr>
<td>2</td>
<td>1.680</td>
<td>0.091</td>
<td>0.050</td>
</tr>
</tbody>
</table>

(Ramasubramaniam and Carter, in progress)

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**HE - Case Study**

- **Material:** AISI 4340 (Q&T) high-strength steel in seawater
  - $E = 210$ GPa
  - $\nu = 0.3$
  - $\sigma_y = 1000 - 1600$ Mpa
  - $N = 0.042 - 0.087$
  - $K_c = 45 - 150$ MPa m$^{1/2}$
  - $\tau_c = 4000 - 6400$ Mpa
  - $V = 7.116 \times 10^{-6}$ m$^3$/mol

- **Impurity (hydrogen)**
  - $D(T_{amb}) = 1.0 \times 10^{-10}$ m$^2$/s
  - $\Delta V = 2.0 \times 10^{-6}$ m$^3$/mol

- **Load:** Applied $P$ (corresp. $K$)

- **Environment**
  - $T = 300-450$ K
  - $C_{eq,0} = 0.1-10$ ppm wt $= 5.5 \times (10^{-6} - 10^{-4})$

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Center crack panel geometry.

Finite-Element Analysis

- Solution method: staggered procedure,

  - At fixed coverage, solve mechanics problem → update stresses, pressure, deformations
  - At fixed pressure, solve diffusion problem → update concentrations

  - BC Crack flanks:
    - Equilibrium impurity coverage on crack flanks: $C = C_{eq}(p)$
    - At the cohesive zone: $J_n = 0$.

  - BC at external boundaries: $C = 0$.
  - IC: $C = C_{eq}(p)$ on crack flanks; $C = 0$ elsewhere.

HE – Hydrogen concentration

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HE – Hydrogen concentration


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HE – Plastic strain

HE – Plastic strain

HE – Propagation velocity

- Calculated curves reproduce existence of threshold $K_{\text{ISCC}}$ and plateau $V_{P,\text{II}}$.
- Trends agree with experiments, considering the large scatter.

HE - Threshold $K_{ISCC}$ vs. $\sigma_y$

- Calculated curve reproduces experimental trend.
- For high $\sigma_y$ calculations approach upper experimental bound.
- Crack morphology changes from transgranular at low $\sigma_y$ to intergranular at high $\sigma_y$.
- At high $\sigma_y$, a stronger effect of H on grain boundaries (not accounted for) would improve agreement. Likewise for $t_i$ vs. $K_i$.

HE - Plateau $V_{P,\parallel}$ vs. $\sigma_y$

- Results for several high strength steels in various media included.
- Calculated curve reproduces experimental trend.
- For high $\sigma_y$, a stronger effect of H on grain boundaries (not accounted for) would improve agreement in slope.
- For low $\sigma_y$ there is a paucity of data. (Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, 52 (2004) 2403)
HE - $V_{P,\|}$ vs. temperature

- Several high strength steels included.
- Calculated curve reproduces increasing (Arrhenius) part.
- Calculated activation energy for $V_{P,\|}$, $Q_V$, is similar to that taken for $D_{\text{eff}}$, $Q_D \approx 40 \text{kJ/mol}$.
- Fall in $V_{P,\|}$ (generally observed) at high $T$ not reproduced.

Concluding remarks

• Multiscale model (chem + mech) predicts well HE in structural steels at low temperatures (< 100ºC)
• Model does not predict well:
  – High-temperature behavior
  – Aluminum alloys
• Unknown unknowns! HELP? HRPC? Others?
• Model still empirical and incomplete at the mesoscale
• Unmodelled length scales:
  – Interaction between dislocations and H:
    • Solution hardening
    • Pipe diffusion
  – Polycrystalline structure: Grains and grain boundaries
• When is enough enough?

Experimental validation, uncertainty quantification!