A multiscale model for fracture and radiation damage in tungsten

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Fraunhofer IWM Freiburg and Halle - Core Competencies

Materials and Component Testing
under condition of use
(temperature, wear, pressure ...) yield significant results for assessment and simulation

Forming
Specific methods to improve forming processes: hot embossing of glass, springback during sheet forming, rolling of wires, forging, powder pressing and sintering

Simulation
The linking of testing and simulation is significant for the outstanding position of Fraunhofer IWM in the simulation of materials, processes and components

Failure Assessment
of manufacturing or in-service related faults in the bases of safety and lifetime concepts

Microstructural Analysis
by high resolution diagnostics and ion beam technologies lead to a sound understanding of the materials microstructure

Modelling
Development of micromechanical models for damage, brittle fracture and thermocyclical stress

Fraunhofer society invested 3 Mio. € into development of MMM-Tools
our current interest in tungsten: drawing of wires

understanding crack nucleation and crack propagation 

by atomistic modelling

Fracture toughness of tungsten in MPa m$^{1/2}$.

<table>
<thead>
<tr>
<th>Crack system</th>
<th>RT exp.</th>
<th>77 K exp.</th>
<th>Atomistic modeling</th>
</tr>
</thead>
<tbody>
<tr>
<td>${100} {010}$</td>
<td>$8.7 \pm 2.5$</td>
<td>$3.4 \pm 0.6$</td>
<td>2.05</td>
</tr>
<tr>
<td>${100} {011}$</td>
<td>$6.2 \pm 1.7$</td>
<td>$2.4 \pm 0.4$</td>
<td>1.63</td>
</tr>
<tr>
<td>${110} {001}$</td>
<td>$20.2 \pm 5.5$</td>
<td>$3.8 \pm 0.4$</td>
<td>2.17</td>
</tr>
<tr>
<td>${110} {1\bar{1}0}$</td>
<td>$12.9 \pm 2.1$</td>
<td>$2.8 \pm 0.2$</td>
<td>1.56</td>
</tr>
</tbody>
</table>

description of
a) screw dislocations
b) brittle to ductile transition


(using Finnis-Sinclair-potential)
cleavage anisotropy in Silicon:

- cracks on the \( \{110\} \) plane
- crack propagation direction: 
  - [-110] easy
  - [001] not observed

common classical potentials (Stillinger-Weber, Tersoff) give wrong predictions.

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atomistic treatment of local disturbances:

- crack tip
- dislocation core
- grain boundary
- laser ablation
- strong disorder
- disorder
- elastic deformation
- nano wires
- radiation damage
- sputtering
- nanoindenter
- cluster impact

Salonen, Nordlund, Keinonen, Wu
Sputtering of divertor Materials C and W
a multiscale problem

→ atomistic processes in nano- and microscale regions
  ▪ far from equilibrium → quantum treatment
  ▪ close to equilibrium → semi-empirical potentials

→ macroscale prescription of Dirichlet or von Neumann boundary conditions (BC)
  far away from the atomistic zone
  ▪ asymptotic stress field or strain field
  ▪ asymptotic temperature field

→ physics outside the atomistic region is only relevant concerning the atomistic BC
  ▪ micro stresses, micro strains
  ▪ nonreflecting BC
  ▪ heat sink
  ▪ thermostat
a multiscale model

QM | CLASS | CONTINUUM ... 

ATOMS | NODES

→ outline of the talk:  
A) coupling of the three different zones
B) choice of the potentials

A: coupling schemes

**FEAt:** Kohlhoff, Gumbsch, Fischmeister, Phil.Mag.A 64, 851 (1991)
**QC:** Tadmor, Ortiz, Phillips, Phil.Mag.A 73, 1529 (1996)
**SMA:** Moseler, Nordiek, Haberland, PRB 56, 15439 (1997)
**CLS:** Broughton, Abraham, Bernstein, Kaxiras, PRB 60, 2391 (1999)
model for atomistic zone: 1-D solid

- atoms interact via 1st and 2nd neighbour potential:
  \[ E_{\text{pot}} = \frac{1}{2} \sum_i [V(x_i - x_{i-1}) + V(x_i - x_{i-2})] \]

substitutional medium

- idea of FEAt, QC, CLS: replace nonlocal force field by 1st neighbour forces (from FEM description for nodes), equal atomic and nodal positions

- SMA: take heavier nodes on simple cubic lattice
coupling:

pot. energy of atom:  
\[ E_i^a = \frac{1}{2} \left( \frac{1}{2} k_1 (x_i-x_{i-1})^2 + \frac{1}{2} k_1 (x_{i+1}-x_i)^2 + \frac{1}{2} k_2 (x_i-x_{i-2})^2 + \frac{1}{2} k_2 (x_{i+2}-x_i)^2 \right) \]

node:  
\[ E_i^c = \frac{1}{2} \left( \frac{1}{2} k_c (x_i-x_{i-1})^2 + \frac{1}{2} k_c (x_{i+1}-x_i)^2 \right) \]

• QC, CLS: \( E_{pot} = \sum_{i>0} E_i^a + \sum_{i<1} E_i^c \) advantage: Hamiltonfct. \( \rightarrow \) isoenergetic dynamics

disadvantage: unbalanced („ghost“) forces

• FEAt: \( E_{pot}^a = \sum_{i>-2} E_i^a \), \( E_{pot}^c = \sum_{i<-2} E_i^c \) disadvantage: no Hamiltonfct. \( \rightarrow \) energy loss in MD

Advantage: forces balanced
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the high-frequency problem

systematic way to derive coupling

- partition displacement:
  \[ u_p = (\ldots, u_4, u_3, u_2, u_1) \]
  \[ u_q = (u_0, u_{-1}, u_{-2}, u_{-3}, \ldots) \]

- equations of motion:
  \[ -m_p \omega^2 \ddot{u}_p(\omega) = \ddot{f}_p(\omega) - \Phi_{pp} \ddot{u}_p(\omega) - \Phi_{pq} \ddot{u}_q(\omega) \]
  \[ -m_q \omega^2 \ddot{u}_q(\omega) = \ddot{f}_q(\omega) - \Phi_{qp} \ddot{u}_p(\omega) - \Phi_{qq} \ddot{u}_q(\omega) \]

- Greens function:
  \[ m_q \omega^2 G_{qq}(\omega) - \Phi_{qq} G_{qq}(\omega) = 1_{qq} \]

- Formal solution:
  \[ \ddot{u}_q(\omega) = \tilde{G}_{qq}(\omega) \left( -\ddot{f}_q(\omega) + \Phi_{qp} \ddot{u}_p(\omega) \right) \]

- Generalized Langevin equation:
  \[ -m_p \omega^2 \ddot{u}_p(\omega) = \ddot{f}_p(\omega) - \Phi_{pp} \ddot{u}_p(\omega) \]
  \[ + \tilde{R}_p(\omega) + \tilde{\Theta}_{pp}(\omega) \ddot{u}_p(\omega) \]

Random force term:
\[ \tilde{R}_p(\omega) = \Phi_{pq} \tilde{G}_{qq}(\omega) \ddot{f}_q(\omega) \]

Friction Kernel:
\[ \tilde{\Theta}_{pp}(\omega) = -\Phi_{pq} \tilde{G}_{qq}(\omega) \Phi_{qp} \]
substitutional medium approach
Moseler et al., PRB 56, 15439 (1997)

new Q medium:

\[-m_Q^* \omega^2 \tilde{u}_Q^*(\omega) = -\Phi_{QP}^* \tilde{u}_P(\omega) - \Phi_{QQ}^* \tilde{u}_Q^*(\omega)\]

coupled to old P zone:

\[-m_P \omega^2 \tilde{u}_P(\omega) = \tilde{f}_P(\omega) - \Phi_{PP}^* \tilde{u}_P(\omega) + \Theta_{PP}^*(\omega) \tilde{u}_P(\omega)\]

\[\Theta_{PP}^*(\omega) = -\Phi_{PQ}^* G_{QQ}^*(\omega) \Phi_{QP}^*\]

dynamic of \(u_P\) after substitution should be the same:

\[-m_P \omega^2 \tilde{u}_P(\omega) = \tilde{f}_P(\omega) - \Phi_{PP}^* \tilde{u}_P(\omega) + \Theta_{PP}^*(\omega) \tilde{u}_P(\omega)\]

\[+ \tilde{R}_P(\omega) + \Delta_{PP}(\omega) \tilde{u}_P(\omega)\]

\[\Delta_{PP}(\omega) = \Theta_{PP}(\omega) - \Theta_{PP}^*(\omega)\]

if SM has the same long wave length (\(\omega=0\)) behaviour:

\[\tilde{\Delta}_{PP}(\omega) = \tilde{\Delta}_{PP}(-i0) + \omega \tilde{\Delta}'_{PP}(-i0) + \frac{1}{2} \omega^2 \tilde{\Delta}''_{PP}(-i0) + \frac{1}{6} \omega^3 \tilde{\Delta}'''_{PP}(-i0) + \ldots\]
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**New equation of motion for P boundary atoms:**

\[
\mathbf{M}_{PP}^* \ddot{\mathbf{u}}_P(t) = \mathbf{f}_P(t) - \Phi_{PP}^* \mathbf{u}_P(t) - \Phi_{PQ}^* \mathbf{u}_Q^*(t) - \mathbf{M}_{PP}^* \beta_{PP} \dot{\mathbf{u}}_P(t) - \mathbf{M}_{PP}^* \beta_{PQ} \dot{\mathbf{u}}_Q^*(t)
\]

### Derivation

\[
\mathbf{M}_{PP}^* = \mathbf{M}_{PP} - \frac{1}{6} \tilde{\Delta}'''_{PP}(-i0) \mathbf{M}_{PP}^{-1} \tilde{\Delta}'_{PP}(-i0)
\]

\[
\beta_{PP} = i \mathbf{M}_{PP}^* \left( \tilde{\Delta}'_{PP}(-i0) + \frac{1}{6} \tilde{\Delta}'''_{PP}(-i0) \mathbf{M}_{PP}^{-1} \Phi_{PP}^* \right)
\]

\[
\beta_{PQ} = i \mathbf{M}_{PP}^* \left( \frac{1}{6} \tilde{\Delta}'''_{PP}(-i0) \mathbf{M}_{PP}^{-1} \Phi_{PQ}^* \right)
\]

### Do the math for the linear chain:

Slave atoms like in FEAt!!!
Test:

Gaussian wave packet in EAM-Cu:

Reflection:

\[
\beta = 0 \quad \beta_{AD}
\]

Brownian dynamics

\[
\frac{\sigma}{a_0}
\]

\[
R
\]
coupling QM to classical

- embedded cluster calculation
- avoid electronic finite size effects
- covalent materials: H termination
- ionic materials: Madelung potential from classical zone
- metals: **bond order potentials**
  
  
B: Choice of the potentials

QM: A bond order potential for tungsten

parametrized tight-binding for the d-electrons

\[ E_{coh} = E_{bond} + E_{rep} \]

captures directional character of covalent bonds

real-space O(N) method

can be used for a large number of atoms

NO BC for electrons required

excellent for embedding
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**Bond part**

$$E_{\text{bond}} = \sum_{i\alpha \neq j\beta} \Theta_{j\beta,i\alpha} H_{i\alpha,j\beta}$$

**Bond orders**

$$\Theta_{i\alpha,j\beta} = \frac{1}{2} \left( N_{i\alpha,j\beta}^+ - N_{i\alpha,j\beta}^- \right) = \sum_{n_{occ}} 2C_{i\alpha}^{(n)} C_{j\beta}^{(n)}$$

Solved **not by diagonalization**

Calculated via Green’s function formalism

$$\Theta_{i\alpha,j\beta} = -\frac{2}{\pi} \lim_{\eta \to 0} \text{Im} \left\{ \int_{-\infty}^{E_F} G_{i\alpha,j\beta} (E + i\eta) \, dE \right\}$$

Using Lanczos algorithm (recursion method)

$$\hat{H} |U_n \rangle = a_n |U_n \rangle + b_n |U_{n-1} \rangle + b_{n+1} |U_{n+1} \rangle$$

**Bond integrals**

Radial parts are functions of interatomic distance

Angular dependencies given by Slater&Koster

Types of bond integrals depend on materials studied

Parametrized according to **ab initio** data

$$G_{i\alpha,i\alpha}(Z) = \frac{1}{Z - a_0 + \frac{(b_1)^2}{Z - a_1 - \frac{(b_2)^2}{Z - a_2 - \frac{(b_3)^2}{\ddots}}}}$$

![DOS graph](image)
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Repulsive part

\[ E_{rep} = E_{env} + E_{pair} \]

environment-dependent term \( E_{env} \)

- captures the s-p orbital overlap repulsion
- introduced to fit the correct Cauchy pressure

pair potential \( E_{pair} \)

- represents the electrostatic interaction between atoms and double counting correction
classical atomistic potentials: Second-Moment-Approximation or EAM (Finnis-Sinclair) (Johnson-Oh)

Interstitials in tungsten
Formation energies in eV predicted by various methods

<table>
<thead>
<tr>
<th>Direction</th>
<th>EAM</th>
<th>FS</th>
<th>BOP</th>
<th>MBPP</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;110&gt;</td>
<td>10.55</td>
<td>9.71</td>
<td>9.41</td>
<td>9.87</td>
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<tr>
<td>&lt;111&gt;</td>
<td>11.87</td>
<td>9.02</td>
<td>10.99</td>
<td>10.18</td>
</tr>
<tr>
<td>C</td>
<td>12.00</td>
<td>8.99</td>
<td>11.00</td>
<td></td>
</tr>
<tr>
<td>&lt;100&gt;</td>
<td>13.79</td>
<td>9.88</td>
<td>11.91</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>13.27</td>
<td>10.06</td>
<td>11.99</td>
<td></td>
</tr>
</tbody>
</table>
Other semi-empirical potentials:

bcc-materials: directional bonding

a) modified embedded atom (Baskes 1991)

or

b) empirical bond order potentials (Abell-Tersoff-Brenner-Type)

See e.g. Pt-potential of Albe, Nordlund, Averback PRB 65,195124 (2002)
efficiency:

<table>
<thead>
<tr>
<th>timing</th>
<th>BOP</th>
<th>100000 µs/atom/step</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EAM</td>
<td>30 µs/atom/step</td>
</tr>
<tr>
<td></td>
<td>CM</td>
<td>2 µs/node/step</td>
</tr>
</tbody>
</table>

(tested with Pentium-4 2Ghz)

→ systems sizes: 1 ns MD on 512 CPUs for one day
BOP: ~2000 atoms
EAM: ~10^7 atoms
CM: ~10^8 nodes
conclusion: hybrid schemes will be important for future large scale MD simulations of energetic events in solids

balance between quantum accuracy ↔ sufficient systems size and statistics

more work has to be done on QM-order-N-schemes

development of reliable empirical BOPs