Simulation: Powerful tool for Microscale Materials Design and Investigation

Dr. Xining Zang
ME 138/ME238

Prof. Liwei Lin
Professor, Dept. of Mechanical Engineering Co-Director, Berkeley Sensor and Actuator Center
The University of California, Berkeley, CA94720

e-mail: lwlin@me.berkeley.edu
http://www.me.berkeley.edu/~lwlin
Time Scale and Length Scale

Multiscale Modeling Framework

- Quantum mechanics, transition state theory
- Molecular dynamics (MD), accelerated MD
- Kinetic Monte Carlo (KMC), coarse-grained KMC
- Computational fluid dynamics
- Process and plant simulation

Modeling and Simulation

**Modeling:** describes the classical scientific method of formulating a simplified imitation of a real situation with preservation of its essential features. In other words, a model describes a part of a real system by using a similar but simpler structure.

**Simulation:** putting numbers into the model and deriving the numerical end-results of letting the model run on a computer. A simulation can never be better than the model on which it relies.
Computational Materials Science

Experiments

Materials Science Question

Model System

Simulation

Result Analysis

Theory

Micro scale
Meso scale
Atomic scale
Electron scale
THE U.S. MATERIALS GENOME INITIATIVE

Meeting Societal Needs
Advanced materials are at the heart of innovation, economic opportunities, and global competitiveness. They are the foundation for new capabilities, tools, and technologies that meet urgent societal needs including clean energy, human welfare, and national security.

Accelerating Our Pace
The U.S. Materials Genome Initiative (MGI) challenges researchers, policymakers, and business leaders to reduce the time and resources needed to bring new materials to market—a process that today can take 20 years or more.

Building Infrastructure for Success
The MGI is a multi-agency initiative to renew investments in infrastructure designed for performance, and to foster a more open, collaborative approach to developing advanced materials, helping U.S. Institutions accelerate their time-to-market.

The Materials Genome Initiative is a multi-agency initiative designed to create a new era of policy, resources, and infrastructure that support U.S. institutions in the effort to discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost.

Advanced materials are essential to economic security and human well being, with applications in industries aimed at addressing challenges in clean energy, national security, and human welfare, yet it can take 20 or more years to move a material after initial discovery to the market. Accelerating the pace of discovery and deployment of advanced material systems will therefore be crucial to achieving global competitiveness in the 21st century.

https://mgi.nist.gov/
Harnessing the power of supercomputing and state of the art electronic structure methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.
Molecular Dynamics

Key: Newton second law & Hamiltonian

\[ \frac{d^2 \mathbf{r}}{dt^2} = \frac{\mathbf{F}}{m} \]

\[ H(r, p) = \frac{|p|^2}{2m} + V(r) \]

\[ \frac{dr}{dt} = \frac{\partial H(r, p)}{\partial p} \]
\[ \frac{dp}{dt} = -\frac{\partial H(r, p)}{\partial r} \]

\[ \frac{dH}{dt} = \frac{\partial H(r, p)}{\partial r} \cdot \frac{dr}{dt} + \frac{\partial H(r, p)}{\partial p} \cdot \frac{dp}{dt} = 0 \]
Molecular Dynamics

• Using the information gained from $r$, $v$ and application of the forces:
  • Initial positions are advanced towards a lower energy state.
    • Through some time step delta $t$
  • New positions are obtained.
  • New velocities are obtained
  • REPEAT.
• This is repeated as many times as is needed to obtained equilibrium.
MD for mechanical properties

- Young’s Modulus
- Yield Strength
- Interface structure
- Dislocation-interface interaction
An example: ultralow elastic modulus

10~20nm thickness, <10nm crystallinity
DFT predict ~400 GPa C11
Tested 20~30GPa elastic modulus
(>one order decrease)
Mechanical property

Nanocrystalline softening

Has been limitedly studied in typical FCC metal Cu/Ti etc

Grain boundary dominated sliding > dislocation strengthening

2D stress field

Reverse Hall-Peige

Need to be tested out


International Journal of Solids and Structures
Volume 49, Issue 26, 15 December 2012, Pages 3942-3952
Why atomistic simulation?

\[ \sigma_f = \sigma_0 + \left[ M \sqrt{3} \theta_{LAB} (1 - f) + k_1 \sqrt{f} \right] D^{-1/2}_B \]

\[ = \sigma_0 + k_2 D^{-1/2}_B \]

- Hall-petch
- thickness <5nm
- Single dislocation
- Nanocrystalline softening?

A.Misra, M.J,Demkowicz,et,al JOM,2008 April
Dislocation


A dislocation is characterized by

1) the Burgers-Vector \( \mathbf{b} \)
2) the direction \( \mathbf{u} \) of the dislocation line

Common "types" of dislocations:

a) edge dislocation \( (\mathbf{b} \cdot \mathbf{u} = 0) \)
b) screw dislocation \( (\mathbf{b} \cdot \mathbf{u} = 1) \)
c) 60° dislocation \( (\mathbf{b} \cdot \mathbf{u} = 0.5) \)
Simulation process outline

Calculation details
- Interface structure
- Dislocation-interface interaction
- Methodology

Results and discussion

Difficulties and questions
Simulation process outline

- Interface construction
- Relaxation [quenching MD]
- Calculation certain properties
Interface structure

**interface**

- Coherent — transparent
- Semi-coherent — half-transparent
- Incoherent interface — opaque

**examples**

- Cu-Ni (Fcc-Fcc)
  - Medyanik 2009
  - Rao 2000
- Cu-Ag (Fcc-Fcc)
  - Hoagland 2002
- Cu-Nb (Fcc-Bcc)
  - Wang, 2008
Incoherent Cu-Nb

Kurdjumov–Sachs (KS)

KS

plane strain adjoining atom layer

\((111)_{Cu} \parallel (110)_{Nb}, <\bar{1}10>_{Cu} \parallel <\bar{1}11>_{Nb}\)

KS$_1$

KS$_2$

KS$_{min}$
Cu and Nb slabs translate minimize the energy

Positions of Cu and Nb not relaxed

Cu and Nb slabs translate minimize the energy

a strained monolayer

3 Cu<110>, 2 Nb<111> 1 Nb<100>

homogeneous in-plane deformation

Requires

- Direction of the monolayer rows A||<110>1
- The rows C || Nb<100>
- d(A) is chosen such that s(C)=s(<100>Nb)
- d(C) is chosen such that s(A)=s(<110>Nb)

Results

- 1 atoms less per 188 atoms
- Energy per atom to create the artificial monolayer 0.03eV/atom
- The A row lies between the valley of Nb<111>
  And the C rows lies between the Nb<100>

M.J.Demkowicz,
Potential for the bi-layer atoms

- Two-body Morse

- EAM, CuNb in CsCl, first-principle using VASP.

\[
\phi_{CuNb}(r) = D_M \left(1 - e^{\alpha_M (r - R_M)} \right) - D_M
\]

\[
\phi'_{CuNb}(r) = \phi_{CuNb}(r) - \phi_{CuNb}(r_{cut}) + \left( \frac{r_{cut}}{m} \right) \left[ 1 - \left( \frac{r}{r_{cut}} \right)^m \right] \left( \frac{d\phi_{CuNb}}{dr} \right)_{r=r_{cut}}
\]

Fitted properties of the EAM interaction potentials used in this study

<table>
<thead>
<tr>
<th>Source of numerical values</th>
<th>(dH(\text{Nb in Cu})(\text{eV}))</th>
<th>(dH(\text{Cu in Nb})(\text{eV}))</th>
<th>(a\text{Cl}) (nm)</th>
<th>(B_{\text{Cl}}) (GPa)</th>
<th>(E^{\text{NaCl}}_{\text{coh}}) (eV)</th>
<th>(E^{\text{ZnS}}_{\text{coh}}) (eV)</th>
<th>(E^{\text{BN}}_{\text{coh}}) (eV)</th>
<th>(m) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EAM 1</td>
<td>1.01</td>
<td>0.49</td>
<td>3.24</td>
<td>173</td>
<td>-4.42</td>
<td>-3.59</td>
<td>-3.28</td>
<td>-0.38</td>
</tr>
<tr>
<td>EAM 2</td>
<td>1.02</td>
<td>0.50</td>
<td>3.23</td>
<td>175</td>
<td>-4.46</td>
<td>-3.62</td>
<td>-3.30</td>
<td>-0.39</td>
</tr>
<tr>
<td>EAM 3</td>
<td>1.00</td>
<td>0.51</td>
<td>3.22</td>
<td>176</td>
<td>-4.51</td>
<td>-3.65</td>
<td>-3.33</td>
<td>-0.40</td>
</tr>
<tr>
<td>EAM 4</td>
<td>1.02</td>
<td>0.48</td>
<td>3.31</td>
<td>168</td>
<td>-4.53</td>
<td>-3.65</td>
<td>-3.33</td>
<td>-0.41</td>
</tr>
<tr>
<td>Experiment/VASP</td>
<td>1.02 [24]</td>
<td>0.48 [24]</td>
<td>3.22</td>
<td>168</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

Details about the structure construction in papers


Cu-Nb Hoagland et.al, Philos. Mag, 2006

Cu-Ni / Cu-Ag Hoagland et.al, Philos. Mag, 2002

Cu-Nb S. Shao, et.al, Model. Sim. MSE 2010

**KS1** region 1 —— region 2

PBC:

in the x and z directions.

Cu: $42 \frac{a_{Cu}}{2} [1\bar{1}\bar{2}] 185.9530 \text{ A ; } 19 \frac{a_{Cu}}{2} [1\bar{1}0] 48.5677 \text{A};$

Nb: $23 \frac{a_{Nb}}{2} [\bar{1}\bar{1}2] 185.9614 \text{ A ; } 17 \frac{a_{Cu}}{2} [\bar{1}1\bar{1}] 48.5958 \text{A};$

**KS2** Cu inserting strained monolayer

**displacement gradient**

\[
\frac{\partial u}{\partial x} = -0.04785 \quad \frac{\partial u}{\partial z} = -0.09209 \quad \frac{\partial w}{\partial x} = 0.02763 \quad \frac{\partial w}{\partial z} = 0.05317
\]

additional PBC **displacement gradient**

\[
\frac{\partial u}{\partial x} = -0.4144e-4 \quad \frac{\partial u}{\partial z} = 0.4867e-3
\]

\[
\frac{\partial w}{\partial x} = -0.1441e-4 \quad \frac{\partial w}{\partial z} = 0.8811e-4
\]
$X, z = 18.6 \text{ nm } y = 4.86$

$K_{s\text{min}}$

Relaxation:
Translate in 3 directions, but rotation is not allowed
Excess energy:
(relative to their respective cohesive energy.)
Another way to construct the interface

Fixing bottom wide enough

Two sets of Slip plane.10.5

dislocations through interface Impossible

Dislocation transmission

Cu-Nb  S. Shao, et.al, Model.Sim.MSE 2010
Interface-dislocation interaction

- Modulus interaction
- Size interaction
- Chemical interaction
- "ω" interaction
Modulus interaction

modulus mismatch (Koehler barrier) introduce an image force

\[ f_k = \left( E^\infty - E^{1-2} \right) / h \]

Koehler stress to move a screw dislocation from a softer layer to a harder layer against its elastic image

\[ \tau_k^* = \frac{\mu_1 (\mu_1 - \mu_2) b}{4\pi (\mu_2 + \mu_1) h} \]

(a/2)<110> screw dislocations are considered to be split into Shockley partials
Size interaction

van der Merwe misfit dislocations /coherency stress

cohereency stress in multilayers:

- lattice parameter misfit between the lamellae,
- elastic constants of the individual lamellae,
- volume fraction of the lamellae and wavelength of the multilayer system

Misfit dislocations —— forest-type obstacles

\[
\tau_d^* = \begin{cases} 
\alpha \mu \left( \frac{\delta a}{a} - b \right) \frac{\lambda}{\lambda_c}, & \lambda > \lambda_c \\
0, & \lambda < \lambda_c 
\end{cases}
\]
Chemical interaction

gamma surface mismatch introduce a localized force on the gliding dislocations

\[ \delta E = \delta E_{el} + \delta E_{ch} \]

\( \delta E_{el} \) the negative elastic interaction energy between the Shockley partials

\( \delta E_{ch} \) the total energy of the stacking fault bounding the partials.

The stress on the leading dislocation of the a pile-up

\[ \tau_{ch}^* = \frac{2\delta\gamma_i}{b} = \frac{\delta\gamma}{b}, \text{where, } \delta\gamma_i = \gamma_i - \gamma_{Cu}, \delta\gamma = (\gamma_{Ni} - \gamma_{Cu}) \]

\( \delta\gamma_i \) the stacking fault energy
Calculation details

- Interface construction
- Relaxation [quenching MD]
- Calculation certain properties
- Relaxation
- Strain related
- Thermodynamic stress
- Elastic constant
- Defect visualization
Interface dislocation displacement field: Barnett-Lothe solution.

field is applied to both the movable and fixed region

Dislocation line is parallel to Z axis

Relaxation Quenching MD until the force on any atom $< 5 \text{pN}$
Lattice glide dislocation enters the interface

disregistry analysis

Pairs of atoms straddle the desired shear plane

relaxed system

\[ r_{ij} = r_i - r_j \]

atoms in the sheared systems

\[ d_{ij} = d_i - d_j \]

The disregistry

\[ r_{ij} - r_{ij} \]
conjugate gradient procedure

energy minimization

parallel atomistic simulation code LAMMPS

visualization of the defects: atomic excess energy, coordinate number;

centro-symmetry parameter

- centro-symmetry parameter:
- Atomeye function to compute P
- pairs of the opposite nearest neighbors

\[
P = \sum_{i=1,\alpha} |R_i + R_{i+\alpha}|^2
\]

\[
C = \frac{\sum_{i=1,\alpha} R_i \cdot R_{i+\alpha}}{\sum_{i=1,\alpha} |R_i + R_{i+\alpha}|^2}
\]

\[
c = \frac{1}{2} \sum_{j=1,2\alpha} |R_j|^2
\]
Indentation lattice glide dislocation

- rigid spherical indenter with radius $R = 40\text{Å}$
- quadratic repulsive force
- center of the top surface

Indentation on Cu-Nb bi-layer
- [adsorption]

Indentation on Nb-Cu bi-layer
- [transmission]
DB 1.45nm from the interface in Cu
• Array relaxed by energy minimization
• Shockley partials $\alpha B D\alpha$

• The lead Shockley partials $\alpha B$ enter the interface leaving trailing Shockley $D\alpha$ in the Cu near original site of DB
• If the Burgers changed into BD, the enters the interface instead
• The observation that one of the partials enters the interface, irrespective of sign, denies the possibility that this response is caused by small residual stresses or coherency stresses local to the interface.
Results and Discussion

- Slip systems in Cu/Nb
- Core spreading of lattice glide dislocation within the interfaces
- Sheared interface attracts lattice glide dislocation Interface
- Interface shear strength
- Elastic interaction between a dislocation and interface