From nano to macro: Introduction to atomistic modeling techniques

Mechanics of Ductile Materials

Lecture 4

Markus J. Buehler
Pair potentials

\[ \phi_i = \sum_{j=1}^{N_{\text{neigh}}} \varphi(r_{ij}) \]

Lennard-Jones 12:6
\[ \varphi(r_{ij}) = 4\varepsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^{6} \right] \]

Morse
\[ \varphi(r_{ij}) = D \{1 - \exp[-\beta(r_{ij} - r_0)]\}^2 \]

Reasonable model for noble gas Ar (FCC in 3D)
Numerical implementation of neighbor search: Reduction of $N^2$ problem to $N$ problem

- Need nested loop to search for neighbors of atom $i$: Computational disaster
- Concept: Divide into computational cells ("bins", "containers", etc.)
- Cell radius $R > R_{\text{cut}}$ (cutoff)

- Search for neighbors within cell atom belongs to and neighboring cells (8+1 in 2D)
- Most classical MD potentials/force fields have finite range interactions

- Other approaches: Neighbor lists
- Bin re-distribution only necessary every 20..30 integration steps (parameter)
"If in some cataclysm all scientific knowledge were to be destroyed and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis that all things are made of atoms - little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another. In that one sentence, you will see there is an enormous amount of information about the world, if just a little imagination and thinking are applied."

--Richard Feynman
Outline

1. **Introduction to Mechanics of Materials**
   Basic concepts of mechanics, stress and strain, deformation, strength and fracture
   Monday Jan 8, 09-10:30am

2. **Introduction to Classical Molecular Dynamics**
   Introduction into the molecular dynamics simulation; numerical techniques
   Tuesday Jan 9, 09-10:30am

3. **Mechanics of Ductile Materials**
   Dislocations; crystal structures; deformation of metals
   Tuesday Jan 16, 09-10:30am

4. **Dynamic Fracture of Brittle Materials**
   Nonlinear elasticity in dynamic fracture, geometric confinement, interfaces
   Wednesday Jan 17, 09-10:30am

5. **The Cauchy-Born rule**
   Calculation of elastic properties of atomic lattices
   Friday Jan 19, 09-10:30am

6. **Mechanics of biological materials**
   Monday Jan. 22, 09-10:30am

7. **Introduction to The Problem Set**
   Atomistic modeling of fracture of a nanocrystal of copper.
   Wednesday Jan 22, 09-10:30am

8. **Size Effects in Deformation of Materials**
   Size effects in deformation of materials: Is smaller stronger?
   Friday Jan 26, 09-10:30am

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Historical references


Outline and content (Lecture 4)

- **Topic:** Fracture and deformation – particularly of crystalline materials (metals, ceramics,..)

- **Examples:** Some MD studies of copper nanocrystals

- **Material covered:** Fundamental dislocation mechanics, energetics of dislocations, stress field around crack, dislocation interactions, basis for MD modeling of metals – EAM potentials

- **Important lesson:** Dislocation as fundamental carrier of plasticity, what goes into MD modeling

- **Historical perspective:** Discovery of dislocations in 1930s and understanding of “strength” of materials
Different crystal symmetries exist, depending on the material considered.

For example, many metals have a cubical structure, such as FCC=face centered cubic

Crystal structure: BCC

BCC
Iron (BCC)

Surface Structure of bcc Crystals

- bcc unit cell (100) face
- bcc unit cell (110) face
- Top view: bcc(111) surface plane e.g. Fe(111)
- Side view: bcc(111) surface plane e.g. Fe(111)

Body Centered Cubic Lattice

- bcc (100) surface plane e.g. Fe(100)
- bcc (110) surface plane e.g. Fe(110)

Figure by MIT OCW.

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Crystal structure: HCP

HCP

Zink

Hexagonal Lattice
Crystal structure and potential

- The regular packing (ordering) of atoms into crystals is closely related to the potential details.
- Several local minima for crystal structures exist, but materials tend to go to the structure that minimizes the energy; often this can be understood in terms of the energy per atomic bond and the equilibrium distance (at which a bond features the most potential energy).

<table>
<thead>
<tr>
<th>N=4 bonds</th>
<th>N=6 bonds per atom</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Square lattice" /></td>
<td><img src="image" alt="Hexagonal lattice" /></td>
</tr>
</tbody>
</table>

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Equation of state

Zinc

Images courtesy of the U.S. Navy.


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Stress versus strain properties: 2D

Stress-strain response

Apply uniaxial strain

Change strain in orthogonal direction so that stress is zero (Poisson effect)

Measure stress vs. strain based on virial stress

Obtain derivatives – $E$, $c_{ijkl}$

Figure by MIT OCW.
Stress versus strain properties: 3D
What controls the strength of materials?

- Puzzled and still puzzles scientists...
- Strength not controlled by single unit cell
- Inhomogeneities are crucial:
  - Flaws, defects...
- Goal: Summarize important crystal defects and their role in deformation
  - Atomistic modeling?
Failure of materials initiates at cracks

Griffith, Irwine and others: Failure initiates at defects, such as cracks, or grain boundaries with reduced traction, nano-voids

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Inglis’ solution: Elliptical hole and hole

\[ \sigma_{yy} = \sigma_0^* \left( 1 + 2 \frac{a}{b} \right) \]

\[ \sigma_{yy} = \sigma_0^* \left( 1 + 2 \sqrt{\frac{a}{\rho}} \right) \]

Stress magnification

Model setup for the Inglis/Kolosov problem.

Plot of stress changes at the edge of elliptical cavities. Normalized maximum stress is \( \sigma_{yy}/\sigma_0^* \); insets at top show ellipse orientations. The dashed horizontal line shows the level of stress change in the plate without a cavity present. Arrow shows stress concentration (3.0) for the circular hole \( a = b \).

Geometry for calculating stress in a plate with a circular hole.

\( F^* \)

\( A/4 \)

\( A/4 \)

\( D = A/2 \)
Other crystallographic defects

- Point defects: Vacancies and interstitials
- Can be produced by plastic deformation

- Vacancy formation energy ca. $E_v \sim 1-3 \text{ eV/atom}$, scale with melting temperature $T_m$:
  $E_v \sim 8kT_m$

- Impurity either substitutional (other atom species on lattice site) or interstitial (non-lattice site)


Figure by MIT OCW.

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Grain boundaries

Grain boundary misfit dislocations

Figure by MIT OCW.


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Ductile versus brittle materials

Glass Polymers
Ice...

Shear load

Copper, Gold

Figure by MIT OCW.

(a)

(b)
Derivation stress field around crack tip

See lecture notes
Asymptotic stress field

\[ \frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0, \]

\[ \frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2\sigma_{r\theta}}{r} = 0. \]

\[ \frac{\partial^2 \epsilon_{\theta\theta}}{\partial r^2} + \frac{2}{r} \frac{\partial \epsilon_{\theta\theta}}{\partial r} - \frac{1}{r} \frac{\partial^2 \epsilon_{r\theta}}{\partial r \partial \theta} - \frac{1}{r^2} \frac{\partial \epsilon_{r\theta}}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2 \epsilon_{rr}}{\partial \theta^2} - \frac{1}{r} \frac{\partial \epsilon_{rr}}{\partial r} = 0. \]

\[ \sigma_{rr} = \frac{1}{r} \frac{\partial \chi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \chi}{\partial \theta^2}, \quad \sigma_{\theta\theta} = \frac{\partial^2 \chi}{\partial r^2}, \quad \sigma_{r\theta} = -\frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial \chi}{\partial \theta} \right) \]

\[ \chi = r^{(\lambda+2)} \left[ A_1 \cos \lambda \theta + B_1 \cos (\lambda + 2) \theta \right] \]

\[ + r^{(\lambda+2)} \left[ A_2 \sin \lambda \theta + B_2 \sin (\lambda + 2) \theta \right] \]
Stress field around a (static) crack

Hoop or opening stress

Maximum principal stress

Figure by MIT OCW.
Deformation of metals: Example

Image removed for copyright reasons.
See: Fig. 4 at http://www.kuleuven.ac.be/bwk/materials/Teaching/master/wg02/l0310.htm.

Image removed for copyright reasons.
See: Fig. 6 at http://www.kuleuven.ac.be/bwk/materials/Teaching/master/wg02/l0310.htm.

http://www.kuleuven.ac.be/bwk/materials/Teaching/master wg02/l0310.htm
Theoretical shear strength

- Perfect crystal: Deformation needs to be cooperative movement of all atoms; the critical shear stress for this mechanism was calculated by Frenkel (1926):

\[ \tau_{th} = \frac{b G}{a 2\pi} \approx \frac{G}{30} \]

- Although this is an approximation, the shear strength measured in experiment is much lower:

\[ \tau_{exp} = \frac{G}{10,000...100,000,000} \]

- Difference explained by existence of dislocations by Orowan, Polanyi and Taylor in 1934
- Confirmed by experiments with whiskers (dislocation free crystals)
Ductile materials are governed by the motion of dislocations: Introduction

Dislocations are the discrete entities that carry plastic (permanent) deformation; measured by “Burgers vector”

http://www.people.virginia.edu/~lz2n/mse209/Chapter7.pdf

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Deformation of a crystal is similar to pushing a sticky tape across a surface:

\[ F \sim \tau \cdot L \]

“homogeneous shear”

\[ F \approx F_{\text{ripple}} \]

“localized slip (ripple)”

\[ L_{\text{crit}} \approx \frac{F_{\text{ripple}}}{\tau} \]

Beyond critical length \( L \) it is easier to have a localized ripple…
Animation: Dislocation motion

Animation online:
http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/illustr/a5_1_1.html

Courtesy of Dr. Helmut Foell. Used with permission.
Geometry of a dislocation (3D view)

Image removed due to copyright restrictions.
See: Fig. 2 at http://www.kuleuven.ac.be/bwk/materials/Teaching/master/wg02/l0310.htm.

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Edge and screw dislocations

Figure by MIT OCW.
Slip direction and plane in FCC

For specific crystals, there are certain directions of Burgers vectors and slip planes that are energetically favored.

FCC:
Slip directions are $\frac{1}{2}<110>$
Glide planes are $\{111\}$

The slip planes and directions are those of highest packing density

Figure by MIT OCW.
Experimental observation

Transmission Electron Micrograph of Dislocations

Grain boundary misfit dislocations

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Figure by MIT OCW.
Geometry of a dislocation (3D view)

- How to model nucleation, propagation of dislocations?
- Particularities in different crystal structures
- Energetics?
- Motion of a dislocation? Eq. of motion? Newton’s laws?
- Interactions?
- …
Sources of dislocations

- Dislocation densities can vary from $10^5$ cm$^{-2}$ in carefully solidified metal crystals to $10^{12}$ cm$^{-2}$ in heavily deformed metals.

- Most metals have dislocations intrinsically present (statistical dislocations), e.g. due to deformation or manufacturing history.

- During deformation, dislocations are nucleated from cracks (see earlier slides), grain boundaries, other dislocations, or surface defects/surfaces.

- Frank-Read sources

http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_3_2.html

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Figure by MIT OCW.
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Deformation mechanisms

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Stacking fault energy

Difficulty of creating a dislocation ($\gamma_{us}$) and moving a dislocation through the crystal ($\gamma_{sf}$)

Calculation of stacking fault energy for different interatomic potentials

Short-range pair potentials have zero SFE!

Figure by MIT OCW.

(Schematic)

Consequence: Only partial dislocations expected

Figure by MIT OCW. After Buehler and Gao, "Ultra large scale atomistic simulations of dynamic fracture," 2006.

(Buehler, 2006)
Partial dislocations

- In FCC, dislocations with Burgers vector [110] split up into two “partial dislocations” with Burgers vector 1/6[112]

\[
\begin{align*}
\text{Energy of the perfect dislocation} & = G \cdot b^2 = G \cdot (a/2<110>)^2 = \frac{G \cdot a^2}{2} \\
\text{Energy of the two partial dislocations} & = 2G \cdot (a/6<112>)^2 = 2G \cdot a^2/36 \cdot (1^2 + 1^2 + 2^2) = \frac{G \cdot a^2}{3}
\end{align*}
\]

Metals with low SFE and materials under geometric confinement often have large stacking faults.
Partial dislocations

Image removed due to copyright restrictions.
Separation of partial dislocations

Width of stacking fault

\[ r_e = \frac{\mu b^2}{8 \pi \gamma_{sf}} \frac{2 - \nu}{1 - \nu} \left( 1 - \frac{2 \nu \cos(2\beta)}{2 - \nu} \right) \sim \frac{1}{\gamma_{sf}} \]

Approaches infinity for \( \gamma_{sf} \to 0 \)
Stress field around a dislocation

• Each dislocation induces a long-range stress field in the crystal

• Around the dislocation core:

Figure by MIT OCW.
Dislocations: Interaction

Important to understand how materials deform

Figure by MIT OCW.

Dislocation Annihilation

(Perfect Crystal)
Nano-confinement of dislocations in ultra thin films on substrates

Figure by MIT OCW.

(Buehler et al., 2006)
Summary: The nature of dislocations

- Dislocations are complex line defects with complicated interaction with each other and other defects and the crystal lattice.
- They are made up out of atoms, but all atoms are not necessary to describe their behavior unless they undergo reactions; long-range interactions.
- Dislocations are critical to understand the behavior of many materials, in particular metals.
- Modeling of atomistic dislocations with realistic material dimensions of micrometers and beyond has so far been elusive.
- Current research efforts are geared towards developing models that describe deformation of materials based on fundamental principles.
- Dislocations also appear in molecular crystals; but their role remains unclear.
Image removed due to copyright restrictions.
Fig. 1 from Gouldstone, Andrew, Krystyn J. Van Vliet, and Subra Suresh. "Nanoindentation: Simulation of defect nucleation in a crystal." Nature 411 (2001): 656.
Atomistic details of dislocation nucleation

- Dislocation nucleation from a traction-free grain boundary in an ultra thin copper film
- Atomistic results depict mechanism of nucleation of partial dislocation

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Chemical bonding in metals
“metallic bonding”

- Bonding between atoms with low electronegativity 1, 2 or 3 valence electrons, therefore there are many vacancies in valence shell.
- When electron clouds overlap, electrons can move into electron cloud of adjoining atoms.
- Each atom becomes surrounded by a number of others in a three-dimensional lattice, where valence electrons move freely from one valence shell to another.
- Delocalized valence electrons moving between nuclei generate a binding force to hold the atoms together

positive ions in a sea of electrons

Thus:
- Electron gas model
- Mostly non-directional bonding, but the bond strength indeed depends on the environment of an atom, precisely the electron density imposed by other atoms

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## Properties of metals

<table>
<thead>
<tr>
<th>Property</th>
<th>Physical/atomic reason</th>
</tr>
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<tbody>
<tr>
<td>High density</td>
<td>Tightly packed FCC, BCC, HCP</td>
</tr>
<tr>
<td>High melting temperature</td>
<td>Strong forces between ion core and delocalized electrons</td>
</tr>
<tr>
<td>Good conductors of heat</td>
<td>Vibration transport via delocalized electrons (+phonons)</td>
</tr>
<tr>
<td>Good electrical conductors</td>
<td>Delocalized electrons (flow in and out)</td>
</tr>
<tr>
<td>Many metals are ductile</td>
<td>Glide (and climb) of dislocations</td>
</tr>
<tr>
<td>Lustrous</td>
<td>Reflection of light by electron gas</td>
</tr>
</tbody>
</table>

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Why pair potentials fail…

- In pair potentials, the strength of each bond is dependent only on the distance between the two atoms involved: The positions of all the other atoms are not relevant (works well e.g. for Ar where no electrons are available for bonding and atoms are attracted with each other only through the weak van der Waals forces)

- However: QM tells that the strength of the bond between two atoms is affected by the environment (other atoms in the proximity)

- As a site becomes more crowded, the bond strength will generally decrease as a result of Pauli repulsion between electrons.
  The modeling of many important physical and chemical properties depends crucially on the ability of the potential to "adapt to the environment"

- Can not reproduce surface relaxation (change in electron density)

http://www.fisica.uniud.it/~ercolessi/forcematching.html © 2007 Markus J. Buehler, CEE/MIT
Modeling attempts: Pair potential

First attempts using pair potentials

\[ \phi_i = \sum_{j=1\ldots N_{\text{neigh}}} \varphi(r_{ij}) \]

Lennard-Jones 12:6

\[ \varphi(r_{ij}) = 4\varepsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right] \]

Morse

\[ \varphi(r_{ij}) = D\{1 - \exp[-\beta(r_{ij} - r_0)]\}^2 \]

Good for noble gas Ar (FCC in 3D)
Numerical implementation of neighbor search: Reduction of $N^2$ problem to $N$ problem

- Need nested loop to search for neighbors of atom $i$: Computational disaster
- Concept: Divide into computational cells ("bins", "containers", etc.)
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- Search for neighbors within cell atom belongs to and neighboring cells (8+1 in 2D)
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- Other approaches: Neighbor lists
- Bin re-distribution only necessary every 20..30 integration steps (parameter)
Modeling attempts: Multi-body potential

- Multi-body potential depend on more than pairs of atoms, but instead also on the environment of each atom
- Important for metals due to existence of “electron gas”

First proposed by Finnis, Sinclair, Daw, Baskes et al. (1980s)

\[
\rho_i = \sum_{j=1}^{N_{neigh}} \pi(r_{ij})
\]

\[
\phi_i = \sum_{j=1}^{N_{neigh}} \frac{1}{2} \phi(r_{ij}) + F(\rho_i)
\]

Electron density at atom \(i\) based on a pair potential:
Numerical implementation of multi-body EAM potential

- Requires two loops over atoms within each cell

Loop 1:
(i) Pair contributions (derivatives and potential)
(ii) Calculate electron density

Loop 2:
(iii) Calculate embedding function and derivatives

\[ \mathbf{F}_i = - \sum_{j \neq i} \left( \phi'(r_{ij}) + [U'(n_i) + U'(n_j)]\rho'(r_{ij}) \right) \frac{r_{ij}}{r_{ij}} \]

Due to additional (i) calculation of electron density and (ii) embedding contribution EAM potentials are 2-3 times slower than pure pair potentials
Stacking fault energy: LJ potential vs. EAM potential

Consequence: Only partial dislocations expected
Increase in computing power
Classical molecular dynamics

10^2 atoms
10^5 atoms
10^6 atoms
10^8 atoms
10^9 atoms
10^{11} atoms

IBM Almaden Spark
BlueGene/L (USA) 70 TFLOP
NASA Ames (USA) 50 TFLOP
Earth Simulator (Japan) 40 TFLOP
LINUX Clusters

"Gigaflop"
"Teraflop"
"Petaflop" computers

Year

Figure by MIT OCW.

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(Buehler et al., to appear 2006)
## Parallel Molecular Dynamics

**Concept:**
- Divide the workload
- No (immediate) long range interaction (only via dynamics)

- Each CPU is responsible for part of the problem
- Atoms can move into other CPUs (migration)
- Need to know topology or the geometric environment on other CPUs (green region)
- **1,000,000,000 particles on 1,000 CPUs: Only 1,000,000 atoms/CPU**

![Diagram showing parallel molecular dynamics with CPU zones of interest and responsibility](image)

*Figure by MIT OCW.*

(after Schiotz)
Implementation of parallelization

- Shared memory systems (all CPUs “see” same memory)
  - OpenMP (easy to implement, allows incremental parallelization)
  - POSIX threads

- Distributed memory systems
  - MPI (=Message Passing Interface)
    Most widely accepted and used, very portable, but need to parallelize whole code at once

- Parallelization can be very tedious and time-consuming and may distract from solving the actual problem; debugging difficult

- **Challenges:** Load balancing, different platforms, input/output, compilers and libraries, modifications and updates to codes, “think parallel” as manager

- **Strategy for your own code:** Find similar code and implement your own problem

Why is large-scale modeling useful?

- Bridging length scales by direct numerical simulation (DNS)
- Understand the behavior of complex many-particle systems, without imposing constraints or boundary conditions
- Discover new physical phenomena, e.g. collective events that involve a large number of particles

Caution:
- Need to make sure that model produces useful results, i.e. includes new scientific content and discoveries
- Pictures may be pretty, but what do we learn?
Modeling of mechanical behavior of materials is highly demanding and requires models with millions and billions of atoms.

- **2000**
  - 1,000,000,000 particles
  - 10 TFLOP computers
  - 0.3 µm

- **2005**
  - 70,000,000,000 particles
  - 70 TFLOP computers
  - 1.2 µm

- **2010**
  - 7,000,000,000,000 particles
  - 1,000 TFLOP computers
  - 5 µm
Case study: Cracking of a copper crystal…

- Critical load for cracking
- What happens when the load becomes large?
- How to analyze the complex data?
- Limitations of modeling…

Figure by MIT OCW.