MSE235 Materials Structure & Properties Lab
Molecular dynamics laboratory: atomic mechanisms of plastic deformation

Alejandro Strachan
School of Materials Engineering
Purdue University
strachan@purdue.edu
What is in this lab?

• Background lecture
  • Lab objectives
  • Introduction to molecular dynamics (MD)
  • Tensile testing of materials

• Pre-lab lecture
  • How to run online MD simulations at nanoHUB.org
  • MD tensile “tests”

• Lab handout
  • Lab activities using nanoHUB
  • Questionnaire
  • Additional activities
Learning objectives

• Develop an atomic picture of plastic deformation in metals
• Understand the orientation of the active slip system with respect to the tensile axis
• Estimate the strength of perfect crystals and compare it polycrystalline samples
• Strain hardening: difference between annealed and cold worked, and nanoscale samples
Experimental tensile testing

Keith Bowman
“An Introduction to Mechanical Behavior of Materials”
What is molecular dynamics?

- Follow the motion (dynamics) of every atom

- Force acting on each atom
  - Depend on the location of other atoms
  - Interactions are determined by electrons (quantum mechanics); these methods are computationally very intensive
  - Inter-atomic potential (this is what we will use here)

\[ V(\{r_i\}) - \nabla_{r_i} V(\{r_i\}) = F_i \]

- Integrate Newton’s equation of motion

\[ \dot{r}_i = u_i \]

\[ \dot{u}_i = \frac{F_i}{m_i} \]
Molecular dynamics: the idea

Initial atomic positions
• Often a perfect crystal (remove atoms to make a nanowire)
• Generated stochastically for amorphous materials

Initial atomic velocities
• Generated stochastically from the Maxwell-Bolzmann distribution

Integrate Newton’s equations of motion numerically

\[
\begin{align*}
\dot{r}_i(t) &= u_i(t) 
\approx \frac{r_i(t + \Delta t) - r_i(t)}{\Delta t} \\
\dot{u}_i(t) &= \frac{F_i(t)}{m_i} 
\approx \frac{u_i(t + \Delta t) - u_i(t)}{\Delta t}
\end{align*}
\]

\[
\begin{align*}
{r}_i(t + \Delta) &= {r}_i(t) + {u}_i(t)\Delta t \\
{u}_i(t + \Delta) &= {u}_i(t) + \frac{F_i(t)}{m_i}\Delta t
\end{align*}
\]

Euler method (accuracy \(\Delta t\))
(very inaccurate - not used)
The structure of an MD program

1. **Initial atomistic model**
   - Initial conditions \([r_i(0), v_i(0)]\)

2. **Energy expression**
   - Energy and forces
   - Calculate forces at current time \([F_i(t)]\) from \(r_i(t)\)

3. **Driver**
   - Equations of motion, thermostats, applied loads, etc.

   - Integrate equations of motion:
     \[ r(t) \rightarrow r(t + \Delta t) \]
     \[ v(t) \rightarrow v(t + \Delta t) \]
     \[ t \rightarrow t + \Delta t \]

   - Save properties

   - **Done?**
     - **No**
     - **Y**

   - Output file

   - **End**
Obtaining properties from MD

Simple averages

\[
\langle V \rangle = \frac{1}{T} \int_0^T V[r(r)] dt
\]

\[
\langle K \rangle = \frac{1}{T} \int_0^T \sum_i N \frac{p_i^2(t)}{2m_i} dt
\]

Temperature ↔ kinetic energy

\[
\left\langle \sum_i^N \frac{1}{2} m v_i^2 \right\rangle = \frac{d}{2} N k T
\]

Dimensionality (usually 3)

Pressure: virial theorem

\[
P V = N k T + \frac{1}{d} \left\langle F(r_{ij}) \cdot r_{ij} \right\rangle
\]
nanoMATERIALS simulation toolkit @ nanoHUB

• General purpose tool for atomistic simulations of materials

Want to learn more about molecular dynamics?

• *Computer Simulation of Liquids* by M. P. Allen and D. J. Tildesley, Oxford University Press, USA (June 29, 1989);


• Online lecture series: Alejandro Strachan, https://nanohub.org/resources/5838
Nanoscale Platinum tensile specimen

Diameter: 2.6 nm

Periodic length: 4.1 nm

Tensile test:
• Elongate the wire at constant rate
• MD simulation will tell us the stress as a function of time
Nanoscale tensile tests: MD results

Platinum nanowire
Radius 1.3 nm

Initial

Strain: 0.075

Strain: 0.1

Eng. Stress (MPa)

Engineering strain
Nanoscale tensile tests: MD results

Strain: 0.075

Strain: 0.1
Nanoscale specimens: larger strains

Platinum nanowire
Radius 1.3 nm

Engineering strain

Eng. Stress (MPa)
Nanoscale vs. macroscopic tensile specimens

- Nanowire has much higher yield stress
  - Dislocations need to be nucleated (requires extra energy)
- No work hardening in nanowire
  - Dislocations do not accumulate inside the nanowire (always near a surface to escape)