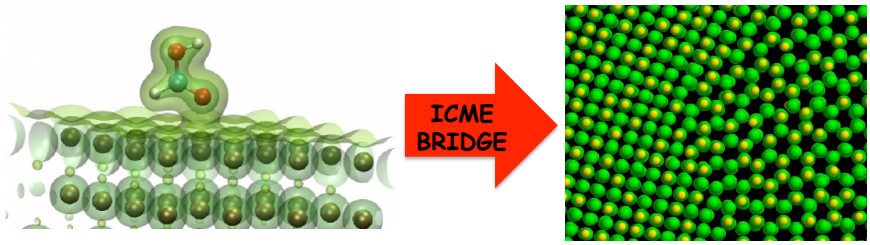
Module 3: LAMMPS Project – Young's Modulus and Peierls Stress of Aluminum

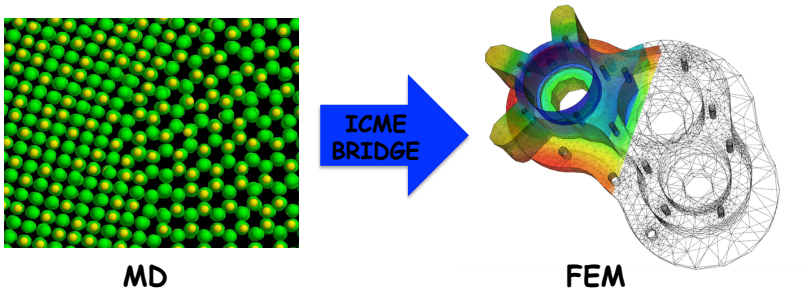
Project Brief

In the spirit of Integrated Computational Materials Engineering (ICME), we have shown how we may use electronic structure calculations to predict the lattice constant for Al, and how this value may – in principle – be used to parameterize a classical force field for Al. This propagation of knowledge from a low level of theory (DFT) to a higher level (MD) is an example of an *ICME bridge*.



http://www.emc2.cornell.edu/content/view/computation-simulation.html
http://www.mse.engin.umich.edu/people/kieffer/projects/multi-scale-molecular-dynamics-simulation-of-self/143

In this project you will use MD simulation to predict continuum level properties of Al – the Young's modulus and Peierls stress – for use in a finite element method (FEM) calculation, building a second ICME bridge from MD to FEM.



http://www.mse.engin.umich.edu/people/kieffer/projects/multi-scale-molecular-dynamics-simulation-of-self/143
http://www.matsim.techfak.uni-erlangen.de/teaching-and-courses/course-descriptors/foundations-of-finite-element-simulation.shtml

Building successive bridges in this manner using the predictions of lower level theory to parameterize higher level theory is the cornerstone of ICME, and offers a means to propagate *ab initio* predictions into continuum models!

Deliverables

You will produce a short report documenting some of your findings and you will submit some of your findings to PrairieLearn. This is indicated in red below and the points allocated for each deliverable are enumerated below. Your report should contain a separate section for each of the tasks listed below, and provide the explicit deliverables requested for each task.

This report will also improve your writing skills: Please make sure that *each* of your paragraphs starts with a "topical sentence" and **format these sentences in bold in your report**. Please make sure that this first sentence (of each paragraph) is concise and "summarizes" the content that follows in the paragraph itself. At the same time, there should be no sentences in any given paragraph that do not align with/elaborate on the "topic" of this first topical sentence. Finally, by reading only these topical sentences, the reader should still understand the story and the logical flow of your report, albeit

without learning any technical details. This structure will be graded and you will lose points if you do not follow it.

Please also note that we will again use peer feedback for this report. Make sure to meet those deadlines, which will be posted on CampusWire. Not sending your report for feedback, or not providing feedback will lead to a 20 point penalty.

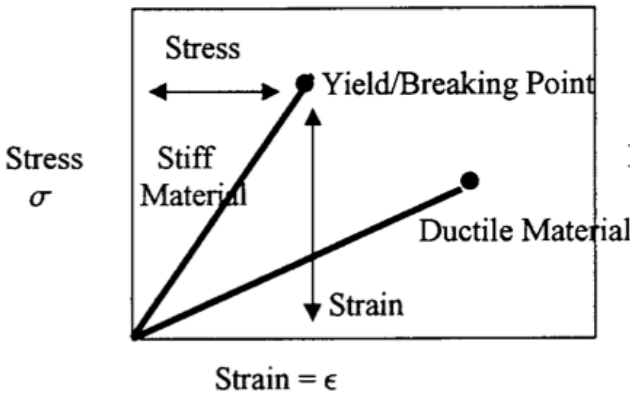
The report should be formatted as a single **single pdf document comprising your report and all requested files**. Submit your report via GradeScope by **11:59pm on 19 October 2020**. **Late submissions will not be accepted.**

The LAMMPS Manual (http://lammps.sandia.gov/doc/Manual.html) and commands list (http://lammps.sandia.gov/doc/Section_commands.html#comm) will be vital to your success.

Part A. Molecular Dynamics Prediction of Young's Modulus of Al.

The Young's modulus (a.k.a. tensile or elastic modulus), *E*, is a measure of the stiffness of a material, and is defined as the ratio of the stress (force per unit area) along a particular axis, σ, divided by the strain (deformation relative to original length) along that axis, $\varepsilon=\Delta L/L_0$, in the regime where this ratio is approximately constant (Hooke's Law holds).

Since the units of strain are dimensionless, *E* has the units of stress (i.e., force per unit area) and can be interpreted as the slope of the stress-strain curve in the linear regime.



$$E = \frac{\text{stress}}{\text{strain}} = \frac{\sigma}{\epsilon} = \frac{\sigma}{\Delta L/L_0}$$

http://www.mbari.org/staff/conn/botany/methods/methods/mmaterial.htm

We can predict the Young's modulus of Al from MD simulations by applying an artificial extensional force to an equilibrated infinite crystal (using the periodic boundaries trick) and recording the observed stress-strain relationship.

A1. Obtain Al EAM potential.

Download the **Al99.eam.alloy** EAM potential from the NIST Interatomic Potentials Repository Project (http://www.ctcms.nist.gov/potentials/).

A2. Construct input script.

Download from the course web site the *partially completed* input script **Al_tensile.in_PARTIAL**. Complete the input script by executing the following tasks.

System Setup

✣ PRAIRIELEARN: Complete the INITIALIZATION block by adding lines for units, dimension, boundary, and atom_style.

Hint: Be careful! What units and atom_style does the EAM potential require?

[4 pts]

✣ PRAIRIELEARN: In the ATOM DEFINITION block, we have defined a variable "latparam" as 4.05 Angstroms – the lattice constant of Al – and used it to construct an fcc lattice in a particular crystallographic orientation.

Using this lattice you should now create a cubic box named "whole" that contains 10 lattice units along each edge and populate it with atoms.

Hint: Be careful – the box side length should be 10 lattice units, not 10 Angstroms!

[3 pts]

The FORCE FIELDS block is complete. There is nothing to do here, but check that you understand everything in this block.

✣ PRAIRIELEARN: In the SETTINGS block, define two computes. One compute should be named "csym" to calculate at every time step the fcc centrosymmetry parameter for each atom. The other should be named "eng" and compute at every time step the potential energy of each atom.

[2 pts]

Equilibration

Now we have initialized our system, but before we can apply an external deformation to record the stress-strain behavior, we must first equilibrate our crystal so that we are starting our simulation from an equilibrated configuration.

✣ PRAIRIELEARN: In the EQUILIBRATION block first reset the timer to zero, define an integration time step of 2 fs, and initialize the atomic velocities from a Maxwell-Boltzmann distribution at 300 K.

Hint: Be careful – what is the unit of time in units "metal"?

[3 pts]

✣ PRAIRIELEARN: Continuing in the EQUILIBRATION block, now define a (*N*, *P*, *T*) fix that will couple the system to a thermostat and barostat to maintain the system at 300 K and 0 bar.

Hint: A good value for the damping parameter in *T* and *P* is 1 ps. A good value for the drag is 1.0.

[1 pts]

Continuing in the EQUILIBRATION block, we see that we have defined a number of variables to write to the file **Al_eq.txt**. You will be using this file to plot trajectories of the approach of our system to equilibrium, so let's leave this intact.

✣ PRAIRIELEARN: Continuing in the EQUILIBRATION block, let's now define a custom thermo to dump to the screen every 500 time steps the following variables: step time cpu cpuremain lx ly lz press pe temp

[2 pts]

✣ PRAIRIELEARN: Continuing in the EQUILIBRATION block, let's now define a dump to write all atom positions to **dump.eq.lammpstrj** every 250 time steps.

[1 pts]

✣ PRAIRIELEARN: Continuing in the EQUILIBRATION block, instruct LAMMPS to perform a 30 ps equilibration run.

[1 pts]

✣ PRAIRIELEARN: Continuing in the EQUILIBRATION block, unfix and undump the fix and dump that you defined.

[2 pts]

To terminate the EQUILIBRATION block we save into a variable "L0" the terminal extent of our equilibrated system in the x direction in preparation for our application of a deformation in this system axis. From the way that we initialized our lattice, this is the [100] crystal direction.

Note the LAMMPS idiom that we have used to save this variable:

```
variable tmp equal "lx"
variable L0 equal ${tmp}
```

we first save "lx" into "tmp", and then evaluate "tmp" to save it into "L0". This guarantees that "L0" stores the value of the internal variable "lx" at a particular instant, and will not change in time.

Deformation

Now that we have equilibrated our crystal, we can move on to the application of an external deformation as an external perturbation to reveal the stress-strain behavior.

✣ PRAIRIELEARN: In the DEFORMATION block, restart the timer to zero and specify a 2 fs time step.

[2 pts]

✣ PRAIRIELEARN: Define a (*N*, *P*, *T*) fix to maintain the temperature at 300 K, but – since we will be deforming in the x-direction – apply pressure coupling anisotropically to maintain the pressure in the y and z-directions at 0 bar and leaving the x-direction uncoupled.

Hint: A good value for the damping parameter in *T* and *P* is 1 ps. A good value for the drag is 1.0.

[1 pts]

In the next section of the DEFORMATION block, we see that we are using the deform fix to apply a deformation to the box in the x-direction to elongate it at a strain rate of 1×10^{10} s^{-1}. Check that you understand all lines in this block before proceeding.

✣ PRAIRIELEARN: The following section defines some output to dump to **Al_deform.txt** that you will use later for plotting. Here we are observing and recording the stress strain behavior over the course of the deformation run. Specifically, we are recording the pressure in GPa in the x, y, and z-directions (i.e., the stress experienced by the material along these axes), and also the strain in the x-direction (i.e., the *relative deformation* of the material in the x-axis). Complete the line

```
variable strain equal
```

to record in this variable the instantaneous value of the strain in the x-direction.
Hint: How can you access the current extent of the system in the x-dimension? Where above have you stored the post-equilibrated extent of the system in the x-dimension?

[1 pts]

✣ PRAIRIELEARN: Continuing in the DEFORMATION block, let's now define a custom thermo to dump to the screen every 500 time steps the following variables: step cpuremain v_strain v_p2 v_p3 v_p4 press pe temp

[2 pts]

✣ PRAIRIELEARN: Continuing in the DEFORMATION block, let's now define a dump to write all atom positions to **dump.deform.lammpstrj** every 125 time steps.

[1 pts]

The next section defines a second dump to a trajectory named **dump.deform_*.cfg** with a more flexible format known as cfg. A separate file is dumped at each time step, replacing the *, for which we request a configuration. The file can hold custom variables including atom positions, forces, energy, centrosymmetry etc.

Hint: Be sure that the name of your computes defined above match those in the cfg dump call.

✣ PRAIRIELEARN: Continuing in the DEFORMATION block, instruct LAMMPS to perform a 20 ps deformation run.

[1 pts]

✣ PRAIRIELEARN: Continuing in the DEFORMATION block, unfix and undump **all** of your fixes and dumps.

[5 pts]

Now perform your LAMMPS run.

A3. Approach to equilibrium.

✣ REPORT: Import the file **Al_eq.txt** recording the approach of the system to equilibrium into Matlab, and plot as a function of time (i) box side length, (ii) pressure, (iii) temperature, and (iv) kinetic, potential, and total energy.

Your plots should possess legibly sized text, labeled axes (variable and units), and appropriately scaled axes. Use the same criteria as in the Quantum Espresso report.

[20 pts]

✣ REPORT: Appealing to your plots, would you say that your system has attained equilibrium within the 30 ps equilibration run? **Justify your answer.**

[5 pts]

A4. Stress-strain behavior.

✣ REPORT: Import the file **Al_deform.txt** recording the observed stress-strain behavior of the system into Matlab, and plot the stress in the x, y, and z-directions as a function of strain.

Your plots should possess legibly sized text, labeled axes (variable and units), and appropriately scaled axes. Use the same criteria as in the Quantum Espresso report.

[20 pts]

✣ REPORT: Appealing to the content of your input script and the behavior of the atoms in the material, provide a **physical rationalization** for the different behavior of the stress x, y, and z-directions.

[15 pts]

✣ REPORT: Over what range of strains do you observe approximately Hookean stress-strain behavior?

[5 pts]

✣ REPORT: Use Matlab or Python to perform a linear least squares fit to this linear region to extract an estimate for the Young's modulus **and** 95% confidence intervals on your estimation.

[15 pts]

✣ REPORT: Find (from an appropriate reference, cite this reference) a value for the experimental Young's modulus of Al. How does your MD prediction compare to the experimental value?

[10 pts]

✣ REPORT: The yield stress is the point of maximum stress marking the end of elastic deformation, and the nucleation of dislocations. What is your MD prediction for the yield strength of Al?

[10 pts]

✣ REPORT: Find (from an appropriate reference, cite this reference) a value for the experimental yield strength of Al. How does your MD prediction compare to the experimental value? If your agreement is poor, can you suggest a rationalization for this observation?

[15 pts]

✣ REPORT: Import **dump.deform_*.cfg** into OVITO and color the atoms according to their fcc centrosymmetry parameter recorded during the simulation and dumped into the cfg trajectory. Provide an image of your system just after the nucleation of the dislocation planes **and** be sure to

supplement your image with a color bar showing the range of the centrosymmetry parameter by dumping the colormap to file using the  button within OVITO and noting its range.

Hint 1: Specify the range of your centrosymmetry color scale from 0 to 12 for a clear visualization.

Hint 2: You can, if you wish, more clearly visualize the dislocation planes by eliminating from the visualization pipeline in OVITO all atoms with centrosymmetry index csym<4.

Hint 3: If you are having trouble setting up the OVITO visualization pipeline, watch the tutorial movie OVITO_project_A4.mov hosted on the course web site for an example.

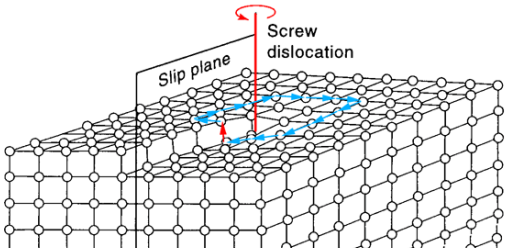
[10 pts]

Part B. Molecular Dynamics Prediction of Peierls Stress for Al.

The *Peierls stress* is the external applied stress required to move a dislocation in an otherwise perfect crystal. The propagation of extant dislocations in a material typically requires a smaller external stress than the homogeneous dislocation nucleation and propagation in a perfect crystal. Macroscopic crystals generically contain dislocations, and their plasticity is therefore controlled by dislocation propagation rather than homogeneous nucleation and propagation.

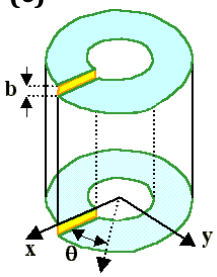
In this study, you will use molecular dynamics simulations to estimate the Peierls stress required to irreversibly move a screw dislocation in the [110] crystal direction. (We choose to study this crystal direction since it contains the smallest Burgers vector, b=√2a, where a is the lattice constant, and therefore requires the smallest Peierls stress to propagate the dislocation. Dislocation motion in this direction will therefore dominate the slip dynamics in the Al crystal.)

(a)

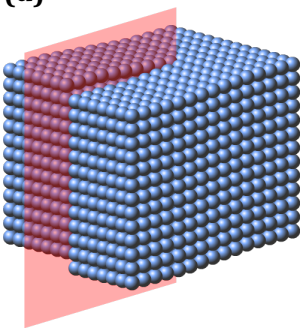


(b)

(c)



(d)



(e)

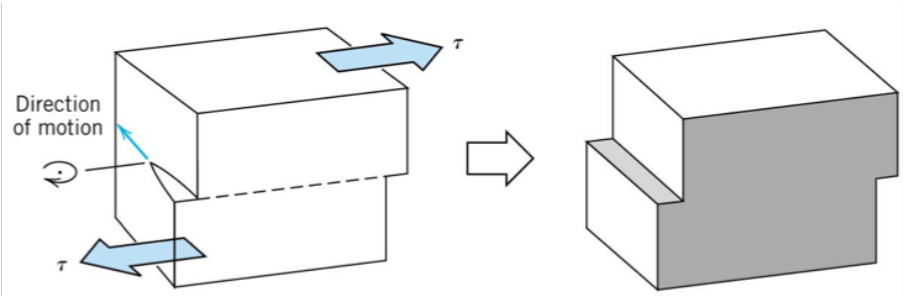


Figure 1. Screw dislocations. **(a)** A screw dislocation in a crystal, illustrating the dislocation core slip plane and Burgers vector, b, in red. The Burgers vector is defined by summing all of the lattice vectors encompassing the dislocation, shown in blue. **(b)** Conceptually, a screw dislocation may be usefully thought of as a tear in a phone book. **(c)** Mathematically, a screw dislocation is defined by a displacement field of the atoms around the screw dislocation core according to the expression $\Delta z = {}^{b}/_{2\pi}\, tan^{-1}({}^{y}/_{x}) = {}^{b\theta}/_{2\pi}$. This displacement field generates what may be thought of as a spiral staircase of atoms that moved up by one Burgers vector every turn. The canonical screw dislocation that we will study herein comprises a Burgers vector equal to the lattice constant. **(d)** An illustration of screw dislocation slip plane shown in pink. **(e)** A screw dislocation is propagated by the application of a shear stress, τ, parallel to the slip plane, causing the dislocation to move perpendicular to the applied stress. The threshold stress required to propagate the dislocation is the Peierls stress.

(a) https://courses.eas.ualberta.ca/eas421/diagramspublic/bergerslarge.gif
(b) http://www.legendarystrength.com/wp-content/uploads/2012/02/Phonebook-Tear.jpg
(c) http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_2_2.html
(d) http://www.spaceflight.esa.int/impress/text/education/Images/Glossary/GlossaryImage%20046.png
(e) Callister & Rethwisch Materials Science and Engineering: An Introduction, 9th ed. (Wiley, 2014)

We shall estimate the Peierls stress by generating a screw dislocation in an otherwise perfect Al crystal then applying a shear stress to the system. The Peierls stress is the stress at which the dislocation first moves.

B1. Obtain Al EAM potential.

Download the **Al99.eam.alloy** EAM potential from the NIST Interatomic Potentials Repository Project (http://www.ctcms.nist.gov/potentials/).

B2. Obtain initial Al crystal configuration.

Download from the course web site the file **restart.eq.FCC_screw110** containing an initial configuration for a 5600 atom Al slab containing a screw dislocation pre-equilibrated to 300 K and 0 bar. The slab measures 38×38×57 Å. It is finite in the x and y-directions, and infinitely replicated in the z-direction through the periodic boundary. The slip plane exists in the x-z plane.

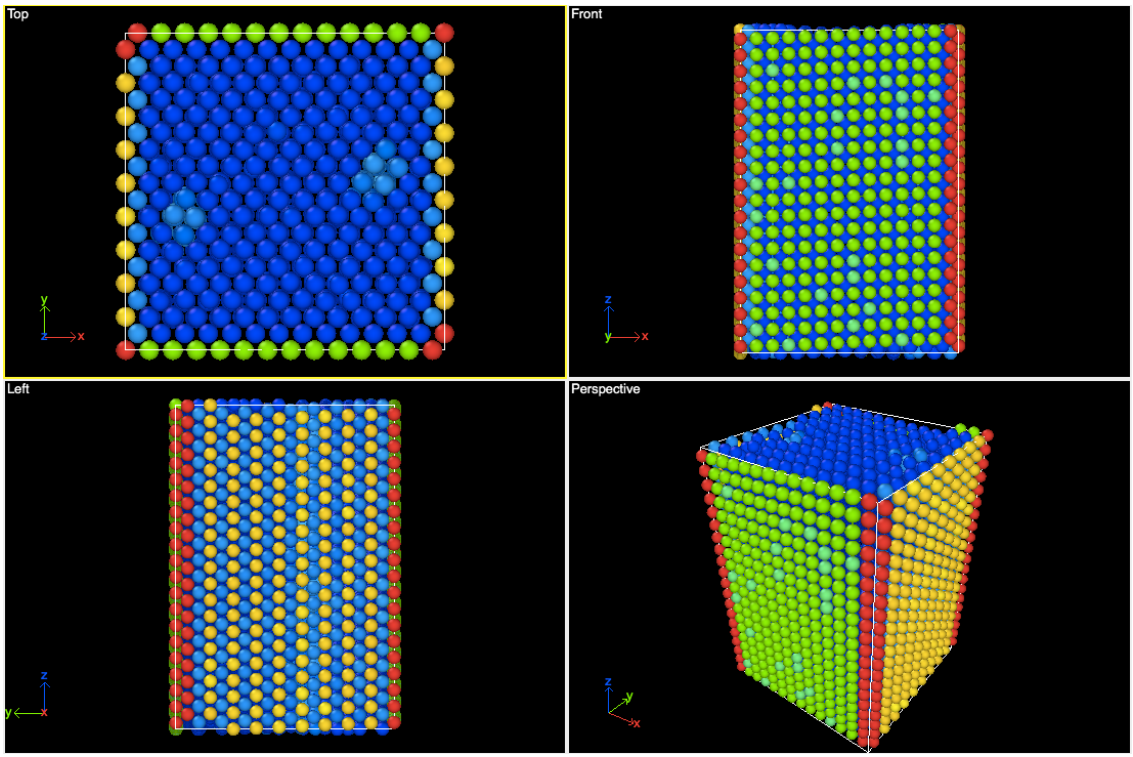


Figure 2. Initial Al crystal configuration held in **restart.eq.FCC_screw110**. The atoms are colored according to their fcc centrosymmetry parameter ranging from 0 (blue) to 40 (red). Observe the pattern of the atoms on the exterior of the slab in the spiral staircase arrangement indicative of a screw dislocation.

B3. Construct input script.

Download from Compass the *partially completed* input script **Al_shear_xz.in_PARTIAL**. Complete the input script by executing the following tasks.

System Setup

✣ PRAIRIELEARN: Complete the INITIALIZATION block by adding lines for units, dimension, boundary, and atom_style.

Hint 1: What units and atom_style does the EAM potential require?

Hint 2: Which directions should be periodic (p), and which should be shrink-wrapped (s)? (Shrink wrapping is positioning of the box face such that all atoms are encompassed – and therefore not lost – no matter how far they move.)

[4 pts]

✣ PRAIRIELEARN: Define within the INITIALIZATION block a variable named "latparam" with a value of 4.05 Å.

[1 pts]

In the ATOM DEFINITION block, we are loading the 300 K and 0 bar equilibrated atomic configuration of the Al block containing a screw dislocation described above. There is nothing to do here, but check that you understand everything in this block.

The FORCE FIELDS block is complete. There is nothing to do here, but check that you understand everything in this block.

✣ PRAIRIELEARN: In the SETTINGS block, define two computes. One compute should be named "csym" to calculate at every time step the fcc centrosymmetry parameter for each atom. The other should be named "eng" and compute at every time step the potential energy of each atom.

[2 pts]

Groups

We ultimately wish to apply an external shear stress to cause the dislocation to move. We will achieve this using a standard trick to apply an external shear stress. We first identify atoms within a two atom thick layer at the exterior of the block (i.e., wall atoms at the edge of the x,y cross section), and define them as the *boundary atoms.* We define the remaining atoms as *core atoms*.

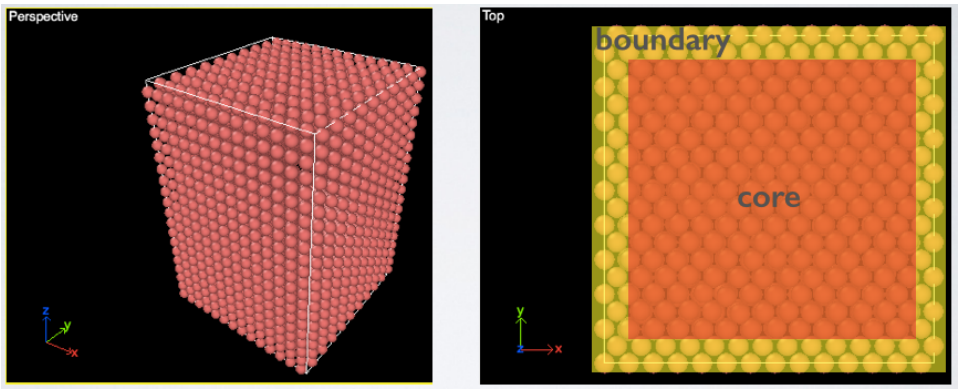


Figure 2. Partitioning of the system into core and boundary atoms.

We then define a molecular dynamics simulation in which the dynamics of the core atoms are propagated normally (i.e., using the Verlet algorithm and possibly a thermostat and/or barostat). The boundary atoms, however, are **not** included in the MD integration scheme, but are instead subjected to a user-defined velocity field. In this case we assign boundary atom z-velocities in direct proportion to their x-distance from the centerline of the block, $v_z \propto -(x - x_{CL})$, and set the x and y-velocities to zero, $v_x = v_y = 0$.

Referring to the right-hand panel of Fig. 2, this causes the wall of boundary atoms on the right side of the image to move down in the z-direction, and the wall of boundary atoms on the left side of the image to move up in the z-direction. The walls of atoms at the top and bottom of the image interpolate between these two extremes, with those precisely on the centerline remaining static. Remember that the periodic boundaries in the z-direction will cause the atoms that exit the high-z top wall to re-enter through the low-z bottom wall!

Importantly, despite partitioning the system into boundary and core atoms, all atoms still interact with all other atoms. In the case of the *boundary atoms*, their interaction with all the other atoms in the system results in a net force on the atom, but we disregard this force in computing the atomic velocity, which is simply assigned by our user-defined field. (This is, of course, highly aphysical!) In the case of the *core atoms*, they continue to interact with one another, and with the boundary atoms.

Accordingly, the relative motion of the boundary atoms at the opposing x-walls of the block has the effect of generating an xz-shear strain, $\varepsilon_{xz} = {}^{\Delta z}/_{L_x}$, to the core atoms, and evolving an associated xz-shear stress, τ_{xz} (Fig. 3). Note that this is the same trick we used in Part A where we applied a *tensile* strain to generate a *tensile* stress, but now a *shear* strain and a *shear* stress.

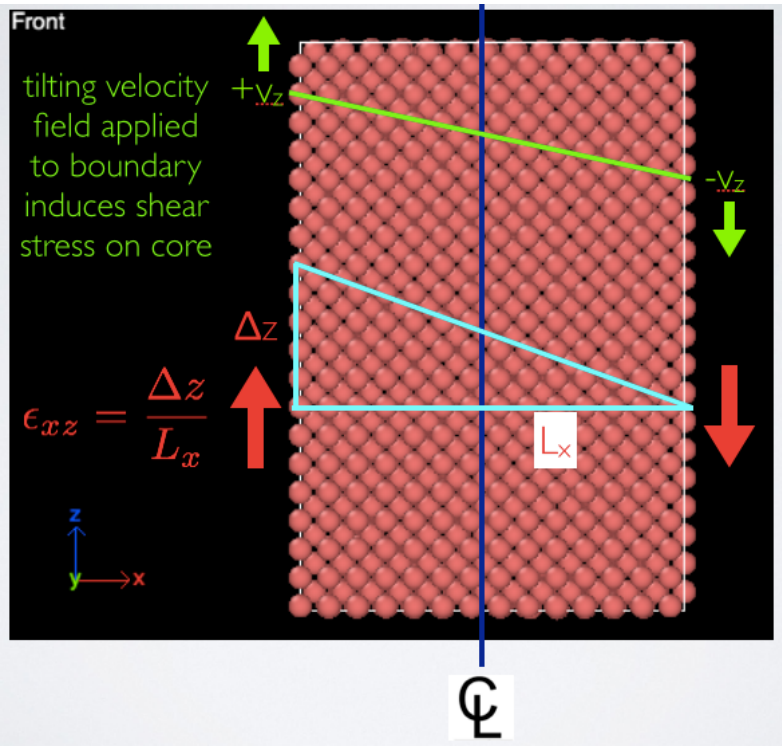


Figure 3. Generation of shear strain and shear stress by application of a user-defined velocity field to the boundary atoms of the Al block.

In the GROUPS block we have exploited the geometry of the lattice to define the x-coordinates of the interior edges of the x-walls, `maxX` and `minX`, and the y-coordinate of the interior edges of the y-walls, `maxY` and `minY` (cf. right panel of Fig. 2). Then using the `region` command, we have defined the regions westWall, eastWall, northWall, and southWall as the low-x, high-x, high-y, and low-y walls respectively.

The `group` commands immediately following take care of establishing each wall region in its own group, all four walls in a group named "boundary", and the remainder of the atoms in a group named "core".

The GROUPS block is complete. There is nothing to do here, but check that you understand everything in this block.

Deformation

✣ PRAIRIELEARN: In the DEFORMATION block, reset the timer to zero and define an integration time step of 2 fs.

[2 pts]

✣ PRAIRIELEARN: Now define a (*N*, *V*, *T*) fix that will couple the ***core atoms only*** to a thermostat system at 300 K. Use a thermostat damping parameter of 0.1 ps and no drag.

N.B. We choose to conduct this calculation in the canonical (*NVT*) ensemble, rather than the isothermal-isobaric (*NPT*) ensemble for simplicity of pressure control. Proper barostatting of a strongly anisotropic system subjected to artificial external forces is a challenge.

[1 pts]

✣ PRAIRIELEARN: The fix labeled 2 applies a user-defined velocity field to the boundary atoms, specifying velocities in x, y, and z by the instantaneous values of the vector variables VX, VY, and VZ holding velocity assignments for all atoms in the system. Immediately preceding this fix, we define the following variables: (i) vperAng – the constant of proportionality between the x-distance of the boundary atom from the centerline of the block and its z-velocity, (ii) VX, (iii) VY, and (iv) VZ. It is your task to complete the lines:

```
variable VX atom
variable VY atom
variable VZ atom
```

Hint 1: Recall from above that $v_x = v_y = 0$ and $v_z \propto -(x - x_{CL})$.

Hint 2: VX, VY, and VZ are vectors of length the number of atoms in the system. Accordingly, they are defined as style "atom".

Hint 3: The internal variable lx can be used to access the instantaneous length of the system in the x-direction.

Hint 4: We can dereference the value of a variable x in an equation assigning a value to another variable as ${x} (cf. http://lammps.sandia.gov/doc/Section_commands.html#cmd_2).

[3 pts]

Continuing in the DEFORMATION block, we see that we have defined a number of variables to write to the file **Al_shear_xz.txt**. You will be using this file to make some stress-strain plots, so let's leave this intact.

✣ REPORT: Before moving on, write a few sentences explaining the following line:

```
variable strain equal "(v_vperAng*lx*time)/lx"
```

[5 pts]

✣ PRAIRIELEARN: Let's now define a custom thermo to dump to the screen every 100 time steps the following variables: step time cpu cpuremain v_strain pxx pyy pzz pxy pxz pyz pe temp

[2 pts]

✣ PRAIRIELEARN: Now define a dump to write all atom positions to **dump.shear_xz.lammpstrj** every 100 time steps.

[1 pts]

✣ PRAIRIELEARN: Instruct LAMMPS to perform a 30 ps run.

[1 pts]

✣ PRAIRIELEARN: Finish up by unfixing and undumping all the fixes and dumps.

[3 pts]

Now perform your LAMMPS run.

B4. Stress-strain behavior.

✣ REPORT: Import the file **Al_shear_xz.txt** recording the observed stress-strain behavior of the system into Matlab or Python. Make two plots: (i) plot **on the same axes** the normal components of the stress – p_{xx}, p_{yy}, p_{zz} – against the xz shear strain, ε_{xz}, (ii) plot **on a new set of axes** the off-diagonal components of the stress – p_{xy}, p_{xz}, p_{yz} – against the xz shear strain, ε_{xz}.

Your plots should possess legibly sized text, labeled axes (variable and units), and appropriately scaled axes. Use the same criteria as in the Quantum Espresso report.

[20 pts]

✣ REPORT: Estimate the value of the Peierls stress for the irreversible movement of a screw dislocation.

Hint 1: Which is the right component of the stress tensor to consider?

Hint 2: The motion of a dislocation will be accompanied with a relaxation in the stress. The first local stress maximum associated with this event is the minimum applied external stress required to move the dislocation.

Hint 3: You may wish to cross-reference your estimation with an OVITO visualization of **dump.shear_xz.lammpstrj**. You should see the dislocation move at the time step corresponding to the strain rate at which the stress is equal to the Peierls stress.

Hint 4: Be careful! You may observe *two* dislocation propagation events. One associated with the propagation of the pre-existing screw dislocation, and one associated with the homogeneous nucleation and propagation of new dislocations. Which will occur at lower values of the stress? Which event corresponds to that associated with a Peierls stress?

[10 pts]

✣ REPORT: Experimental measurements of the Peierls stress for a screw dislocation in Al are all over the map, ranging from 10^{0}-10^{-4} GPa. A detailed MD study employing a modern EAM potential determined a value of 256 MPa [Shin & Carter Phys. Rev. B 88, 064106 (2013)]. How does your MD prediction compare to this value?

[10 pts]

✣ REPORT: Import **dump.shear_xz.lammpstrj** into OVITO for visualization. Have OVITO compute the centrosymmetry parameter appropriate to an fcc crystal (# neighbors = 12), and color the atoms according to the value of this parameter. Eliminate from your visualization all those atoms with centrosymmetry parameter values less than 4 to more clearly see the dislocations within your slab.

Generate a 3D image looking at an angle down through your slab such that the dislocations in the z-direction are visible and generate a **two panel figure** (i) the left panel should show your system in its initial configuration, (ii) the right panel should show your system *after* the irreversible motion of the pre-existing dislocations, but *before* the onset of homogeneous dislocation nucleation. Be sure to supplement your image with a color bar showing the range of the centrosymmetry parameter by dumping the colormap to file using the  button within OVITO and noting its range.

[20 pts]
