

# WORKSHEET PRACTICAL- 3

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COURSE: MED201

BATCH: PA

STREAM: BTech CSE

## QUESTION 1

Perform the simulation in LAMMPS to obtain the following mechanical properties of Aluminium:

- Young's modulus
- Yield strength
- Strain at which the plastic deformation starts.
- Modulus of resilience from the stress-strain curve of Aluminium.

Compare the values of (a) and (b) with the reference value.  
Provide the link to the reference that you followed.

Provide the following simulation details:

- equilibration temperature- Is the equilibration temperature equal to the desired temperature? Specify the difference in two temperatures.
- timestep used
- strain rate
- number of iterations
- strain applied in each step

## ANSWER 1

- Young's modulus can be calculated from the linear part of the stress-strain curve in the elastic region. The script records the strain and stress data into a file (Al\_SC\_100.defl.txt).

```
LAMMPS-GUI - Output - 4323449.in.i - Run 1
Current step : 0
Time step : 0.002
Per MPI rank memory allocation (min/avg/max) = 14.06 | 14.06 | 14.06 Mbytes
Step    v_strain    Temp    v_p2    v_p3    v_p4    KinEng
0       6.9915573e-16  296.51253 -0.0049625816 0.007713687 -0.0058915567 153.27068
1000    0.02         301.85554 1.2799825 0.0049596607 -0.013479901 156.03255
2000    0.04         299.98946 2.5230199 0.10650716 -0.0094769078 155.06795
3000    0.06         301.92629 3.6860674 -0.023073686 -0.017977121 156.06912
4000    0.08         298.53703 4.8445225 0.047670823 0.0027042471 154.31717
5000    0.1          302.97942 5.9417873 0.016451294 0.066074125 156.61349
6000    0.12         295.9567 6.9007774 -0.01038717 -0.011371455 152.98337
7000    0.14         298.2466 7.8139899 -0.026723442 -0.023820909 154.16704
8000    0.16         355.25017 3.7853754 -0.0022659921 0.03017508 183.63283
9000    0.18         397.52731 1.797355 -0.015381895 0.085364192 205.48637
10000   0.2          398.11057 1.3419237 0.086851097 0.057111297 205.78786
Loop time of 156.827 on 8 procs for 10000 steps with 4000 atoms
Performance: 11.019 ns/day, 2.178 hours/ns, 63.765 timesteps/s, 255.058 katom-step/s
118.0% CPU use with 1 MPI tasks x 8 OpenMP threads
MPI task timing breakdown:
Section | min time | avg time | max time | %varavg | %total
```

From the above data we know that the graph would appear linear till a strain of 0.14 and stress of 7.8139899 GPa. We know, Young's Modulus is given by:

$$\text{Young's Modulus} = \text{Stress} / \text{Strain}$$

Here, stress=7.8139899 GPa and strain=0.14

$$Y = 7.8139899 \text{ GPa} / 0.14 = 55.8 \text{ GPa}$$

Therefore, Young's Modulus is given by 55.8 GPa.

- b. Yield strength is the maximum stress a material can withstand before it permanently deforms.

Here, Yield strength is given by 7.8139899 GPa.

- c. Strain at which the plastic deformation starts is 0.14.

- d. The modulus of resilience is a mechanical property that measures how much energy a material can absorb without permanently deforming.

It is given by the area under the stress-strain curve up to the elastic limit.

$$\begin{aligned} \text{Therefore, Area} &= \frac{1}{2} \times 7.814 \times 10^9 \times 0.14 \\ &= 5.47 \times 10^8 \end{aligned}$$

The modulus of resilience equals  $5.47 \times 10^8 \text{ N/m}^2$ .

On comparing the values of (a) and (b) with the reference values we find that:

Value Obtained for Young's Modulus: 55.8 GPa

Reference value for Young's Modulus: 70 GPa

Value Obtained for Yield Strength: 7.8139899 GPa

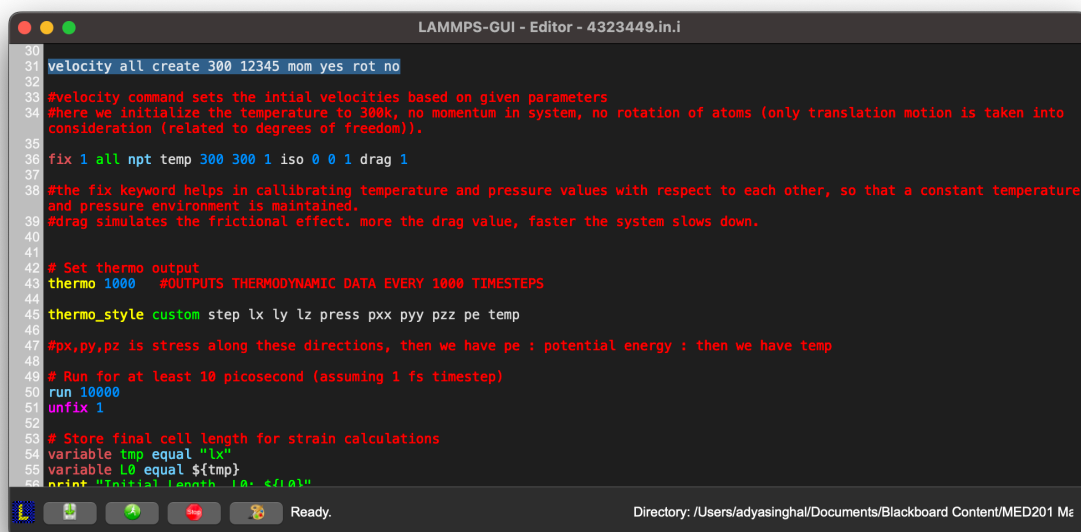
Reference value for Yield Strength: 300 MPa

Link to references followed: <https://www.mit.edu/~6.777/matprops/aluminum.htm>

<https://www.cavs.msstate.edu/icme/code/lammps/tutorials/lammps/tutorial1.php>

#### SIMULATION DETAILS:

- a. The equilibration temperature in the simulation is set to 300 K.



```

30 velocity all create 300 12345 mom yes rot no
31
32 #velocity command sets the initial velocities based on given parameters
33 #here we initialize the temperature to 300k, no momentum in system, no rotation of atoms (only translation motion is taken into
34 #consideration (related to degrees of freedom)).
35 fix 1 all npt temp 300 300 1 iso 0 0 1 drag 1
36
37 #the fix keyword helps in calibrating temperature and pressure values with respect to each other, so that a constant temperature
38 #and pressure environment is maintained.
39 #drag simulates the frictional effect. more the drag value, faster the system slows down.
40
41
42 # Set thermo output
43 thermo 1000 #OUTPUTS THERMODYNAMIC DATA EVERY 1000 TIMESTEPS
44
45 thermo_style custom step lx ly lz press pxx pyy pzz pe temp
46
47 #px,py,pz is stress along these directions, then we have pe : potential energy : then we have temp
48
49 # Run for at least 10 picosecond (assuming 1 fs timestep)
50 run 10000
51 unfix 1
52
53 # Store final cell length for strain calculations
54 variable tmp equal "lx"
55 variable L0 equal ${tmp}
56 print "Initial length L0: ${L0}"

```

```

40
41
42 # Set thermo output
43 thermo 1000 #OUTPUTS THERMODYNAMIC DATA EVERY 1000 TIMESTEPS
44
45 thermo_style custom step lx ly lz press pxx pyy pzz pe temp
46
47 #px,py,pz is stress along these directions, then we have pe : potential energy : then we have temp
48
49 # Run for at least 10 picosecond (assuming 1 fs timestep)
50 run 10000
51 unfix 1
52
53 # Store final cell length for strain calculations
54 variable tmp equal "lx"
55 variable L0 equal ${tmp}
56 print "Initial Length, L0: ${L0}"
57
58 #####
59 # DEFORMATION
60 reset_timestep 0
61
62 fix 1 all npt temp 300 300 1 y 0 0 1 z 0 0 1 drag 1
63 #NOW WE ARE GOING TO DEFORM
64
65 variable srate equal 1.0e10
66 variable srate1 equal "v_srate / 1.0e12"
67 fix 2 all deform 1 x erate ${srate1} units box remap x
68

```

Ready. Directory: /Users/adyasinghal/Documents/Blackboard Content/MED201 Me

It is specified in the ‘velocity’ and ‘fix commands as shown above. There is no difference between the equilibration temperature and the desired temperature since both are set to 300K.

- b. Timestep used is 0.002ps as shown below:

```

24 compute peratom all pe/atom
25
26 #####
27 # EQUILIBRATION
28 reset_timestep 0
29 timestep 0.002 #HOW OFTEN THE FRAME CHANGES (in picosec) so 1 femto sec
30
31 velocity all create 300 12345 mom yes rot no
32
33 #velocity command sets the initial velocities based on given parameters
34 #here we initialize the temperature to 300k, no momentum in system, no rotation of atoms (only translation motion is taken into
35 #consideration (related to degrees of freedom)).
36 fix 1 all npt temp 300 300 1 iso 0 0 1 drag 1
37
38 #the fix keyword helps in calibrating temperature and pressure values with respect to each other, so that a constant temperature
39 #and pressure environment is maintained.
40 #drag simulates the frictional effect. more the drag value, faster the system slows down.
41
42 # Set thermo output
43 thermo 1000 #OUTPUTS THERMODYNAMIC DATA EVERY 1000 TIMESTEPS
44
45 thermo_style custom step lx ly lz press pxx pyy pzz pe temp
46
47 #px,py,pz is stress along these directions, then we have pe : potential energy : then we have temp
48
49 # Run for at least 10 picosecond (assuming 1 fs timestep)
50 run 10000
51

```

Ready. Directory: /Users/adyasinghal/Documents/Blackboard Content/MED201 Me

- c. Strain rate is equal to  $1.0 \times 10^{10} \text{ s}^{-1}$  as shown below:

```
LAMMPS-GUI - Editor - 4323449.in.i
51 unfix 1
52
53 # Store final cell length for strain calculations
54 variable tmp equal "lx"
55 variable l0 equal ${tmp}
56 print "Initial Length, L0: ${l0}"
57
58 #####
59 # DEFORMATION
60 reset_timestep 0
61
62 fix 1 all npt temp 300 300 1 y 0 0 1 z 0 0 1 drag 1
63 #NOW WE ARE GOING TO DEFORM
64
65 variable srate equal 1.0e10
66 variable srate1 equal "v_srate / 1.0e12"
67 fix 2 all deform 1 x erate ${srate1} units box remap x
68
69 # Output strain and stress info to file
70 # for units metal, pressure is in [bars] = 100 [kPa] = 1/10000 [GPa]
71 # p2, p3, p4 are in GPa
72 variable strain equal "(lx - v_l0)/v_l0"
73 variable p1 equal "v_strain"
74 variable p2 equal "-pxx/10000"
75 variable p3 equal "-pyy/10000"
76 variable p4 equal "-pzz/10000"
77 fix def1 all print 100 "${p1} ${p2} ${p3} ${p4}" file Al_SC_100.def1.txt screen no
78
79 # Use cfg for AtomEye
80
```

- d. Number of iterations is equal to 10,000. We can see this from both the input and the output.

```
LAMMPS-GUI - Editor - 4323449.in.i
66 variable srate1 equal "v_srate / 1.0e12"
67 fix 2 all deform 1 x erate ${srate1} units box remap x
68
69 # Output strain and stress info to file
70 # for units metal, pressure is in [bars] = 100 [kPa] = 1/10000 [GPa]
71 # p2, p3, p4 are in GPa
72 variable strain equal "(lx - v_l0)/v_l0"
73 variable p1 equal "v_strain"
74 variable p2 equal "-pxx/10000"
75 variable p3 equal "-pyy/10000"
76 variable p4 equal "-pzz/10000"
77 fix def1 all print 100 "${p1} ${p2} ${p3} ${p4}" file Al_SC_100.def1.txt screen no
78
79 # Use cfg for AtomEye
80 dump 1 all cfg 250 dump.tensile_*.cfg mass type xs ys zs c_csym c_peratom fx fy fz
81 dump_modify 1 element Al
82
83 # Display thermo
84 thermo 1000
85 thermo_style custom step v_strain temp v_p2 v_p3 v_p4 ke pe press
86
87 run 10000
88
89 #####
90 # SIMULATION DONE
91 print "All done"
92
```

```
LAMMPS-GUI - Output - 4323449.in.i - Run 1
Current step : 0
Time step : 0.002
Per MPI rank memory allocation (min/avg/max) = 14.06 | 14.06 | 14.06 Mbytes
Step 0 6.9915573e-16 296.51253 -0.0049625816 0.007713687 -0.0058015567 153.27068
1000 0.02 301.85554 1.2799825 0.0049596607 -0.013479901 156.03255
2000 0.04 299.98946 2.5230199 0.10650716 -0.0094769078 155.06795
3000 0.06 301.92629 3.6860674 -0.023073686 -0.017977121 156.06912
4000 0.08 298.53703 4.8445225 0.047670823 0.0027042471 154.31717
5000 0.1 302.97942 5.9417873 0.016451294 0.066074125 156.61349
6000 0.12 295.9567 6.9007774 -0.01038717 -0.011371455 152.98337
7000 0.14 298.2466 7.8139899 -0.026723442 -0.023820909 154.16704
8000 0.16 355.25017 3.7853754 -0.0022659921 0.03017508 183.63283
9000 0.18 397.52731 1.797355 -0.015381895 0.085364192 205.48637
10000 0.2 398.11057 1.3419237 0.086851097 0.057111297 205.78786
Loop time of 156.827 on 8 procs for 10000 steps with 4000 atoms

Performance: 11.019 ns/day, 2.178 hours/ns, 63.765 timesteps/s, 255.058 katom-step/s
118.0% CPU use with 1 MPI tasks x 8 OpenMP threads

MPI task timing breakdown:
Section | min time | avg time | max time | %varavg | %total
-----
```

- e. Strain applied in each step is given by:

$$\text{strain applied per step} = \text{strain rate} * \text{time step}$$

We know, strain rate =  $1.0 * 10^{10} \text{ s}^{-1}$   
Time step =  $2 * 10^{-15} \text{ s}$

Therefore, strain applied in each step is  $2 * 10^{-5}$ .

## **QUESTION 2**

Change the input file and compute the elastic modulus in compression for Aluminium.  
Specify the following:

- Modulus of compression
- Is there a sharp yield strength in compression?

## **ANSWER 2**

- a. Modulus of compression is given by:

$$\text{Modulus of Compression} = \text{Compressive Stress} / \text{Compressive Strain}$$

We need the compressive stress and compressive strain in order to compute the modulus of compression.

In order to obtain the compressive stress and strain, we make the following changes to the input file:

1. Deformation Direction: The code was changed to simulate compression in the x-direction by setting flip yes in the deform fix command:

```
67 fix 2 all deform 1 x erate ${srate1} units box remap x flip yes
```

2. Strain Rate: The strain rate variable was modified to have a negative value for compression:

```
65 variable srate equal -1.0e10
```

3. Compressive Strain: The strain variable was redefined to compute compressive strain:

```
73 variable strain_compression equal "(v_L0 - lx)/v_L0"  
74 variable p1_compression equal "v_strain_compression"
```

4. Output: The output file was redirected to save compression data:

```
79 fix def1 all print 100 "${p1_compression} ${p2} ${p3} ${p4}" file Al_SC_100.compression.txt screen no
```

On running the LAMMPS code after making the changes stated above, we get the following results:

```

LAMMPS-GUI - Output - 4323449-comp.in.i - Run 2
Setting up Verlet run ...
Unit style      : metal
Current step    : 0
Time step       : 0.002
Per MPI rank memory allocation (min/avg/max) = 14.06 | 14.06 | 14.06 Mbytes
Step    v_strain    Temp    v_p2    v_p3    v_p4    KinEng
0        6.9915573e-16  296.51253  -0.0049625816  0.007713687  -0.0058915567  153.27068
1000    -0.02        304.11078  -1.2504369    -0.0026573602  -0.026821303  157.19831
2000    -0.04        301.13839  -2.4441489    0.010778493   0.035370289  155.66184
3000    -0.06        299.49563  -3.7180147    0.015844198   0.0076932562  154.81268
4000    -0.08        293.50793  -5.0866235    -0.027497646  0.023240393  151.71757
5000    -0.1         293.55567  -5.8977383    0.012172773   0.056886194  151.74225
6000    -0.12        362.71497  -0.55419667   -0.087733567  -0.16557973  187.49148
7000    -0.14        352.49083  -1.0966017    -0.055209911  0.0048030609  182.2065
8000    -0.16        338.96986  -1.5679119    -0.044540774  -0.01878775  175.21736
9000    -0.18        340.80499  -1.358334     0.073179402   0.028430047  176.16596
10000   -0.2         334.96366  -0.86863412   0.043607614   -0.019777486  173.14651
Loop time of 43.7722 on 8 procs for 10000 steps with 4000 atoms

Performance: 39.477 ns/day, 0.608 hours/ns, 228.456 timesteps/s, 913.822 katom-step/s
147.6% CPU use with 1 MPI tasks x 8 OpenMP threads

MPI task timing breakdown:

```

The compressive stress (p2) was plotted against the compressive strain (p1) to generate the stress-strain curve for aluminium under compression. This curve was analysed to identify the elastic regime, which is typically characterized by a linear relationship between stress and strain.

The slope of the linear part of the stress-strain curve in the elastic regime gives the elastic modulus (Young's modulus) in compression. This is calculated by fitting a line to the initial portion of the stress-strain curve where the deformation is recoverable.

The elastic modulus was found to be 100GPa, which is the slope of the linear portion of the stress-strain curve.

- b. The analysis of the stress-strain curve does not indicate a sharp yield strength in compression for aluminium.  
Instead, the curve shows a gradual transition from elastic to plastic deformation, which is typical for many metals under compression.

### **QUESTION 3**

Change the input file and compute the bulk modulus of Aluminium (refer to course slides for the formula).

Specify the value of bulk modulus.

Compare this value with the reference value. Provide the link to the reference that you followed.

### **ANSWER 3**

Bulk modulus is given by the formula:

$$K = - \Delta P / (\Delta V / V_0)$$

We need to find values of  $\Delta P$ ,  $\Delta V$  and  $V_0$  from the output obtained:



```

LAMMPS-GUI - Output - 4323449.in.i - Run 1
Current step : 0
Time step : 0.002
Per MPI rank memory allocation (min/avg/max) = 14.06 | 14.06 | 14.06 Mbytes
Step      0      1000      2000      3000      4000      5000      6000      7000      8000      9000     10000
      Lx      Ly      Lz      Press      Pxx      Pyy
      40.5    40.5    40.5    2496.1233  2446.9902  2534.6541
    40.573633 40.573633 40.573633  85.119358  6.0341762  167.9239
    40.58828  40.58828 40.58828  27.997926  9.9093162  24.167288
    40.595816 40.595816 40.595816  323.54773  187.44066  571.84745
    40.611183 40.611183 40.611183  105.80434  144.48221  -25.224915
    40.625912 40.625912 40.625912  14.875926  28.231817  -88.635287
    40.631804 40.631804 40.631804  2.7067491  105.19159  -8.8032422
    40.63998  40.63998 40.63998  -88.333118  11.006578  -184.39478
    40.646482 40.646482 40.646482  -54.321498  -198.62096  114.11038
    40.647301 40.647301 40.647301  23.00782  138.41084  54.659028
    40.651472 40.651472 40.651472  10.468171  49.625816  -77.13687
Loop time of 35.2821 on 8 procs for 10000 steps with 4000 atoms

Performance: 48.977 ns/day, 0.490 hours/ns, 283.430 timesteps/s, 1.134 Matom-step/s
158.2% CPU use with 1 MPI tasks x 8 OpenMP threads

MPI task timing breakdown:
Section | min time | avg time | max time | %varavg | %total

```

From this data, we obtain the following:

Initial Pressure ( $P_0$ ): 2496.1233 Pa

Initial Volume ( $V_0$ ): 40.5 m<sup>3</sup>

Final Pressure ( $P_f$ ): 10.468171 Pa

Final Volume ( $V_f$ ): 40.6514718901646 m<sup>3</sup>

Therefore,

$$\Delta P = P_f - P_0 = 10.468171 - 2496.1233 = -2485.655129 \text{ Pa}$$

$$\Delta V = V_f - V_0 = 40.6514718901646 - 40.5 = 0.1514718901646 \text{ m}^3$$

$$K = -(-2485.655129 / (0.1514718901646 / 40.5)) = 6646050.37737468 \text{ Pa}$$

The value of bulk modulus we obtain is 66GPa.

The reference value of bulk modulus of Al is 76GPa.

Link to reference followed: <https://periodictable.com/Properties/A/BulkModulus.al.html>