Interatomic Potentials of Face Center Cubic Platinum

CHEN 4880 Atomistic Simulations

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For this project we used the LAMMPS simulation tool on nanoHUB.org. We were provided five files that were used thought this project which are listed in Table 1 of Appendix A. A screenshot of each files code can be seen in Figure 1 through Figure 9 of Appendix A.

Problem 1:

Aa) The first method we used to calculate the lattice constant and total energy was the Lennard Jones potential with a built-in minimizer that relaxed the system. This was provided to us in file "lmp-in.1a-relax" which can be seen in Figure 1 of Appendix A. We set the program to start with a lattice constant of 4 angstrom and ran the program. The results are shown in Table 1 below:

Table 1: Results from lmp-in.1a-relax

Step	Potential Energy (eV)	Lx (Angstrom)	Ly (Angstrom)	Lz (Angstrom)
0	-6.564429	4	4	4
1	-6.572252	3.996	3.996	3.996
2	-6.579738	3.992	3.992	3.992
3	-6.58688	3.988	3.988	3.988
4	-6.59367	3.984	3.984	3.984
5	-6.6001	3.98	3.98	3.98
6	-6.606161	3.976	3.976	3.976
7	-6.611845	3.972	3.972	3.972
8	-6.617144	3.968	3.968	3.968
9	-6.622049	3.964	3.964	3.964
10	-6.626551	3.96	3.96	3.96
11	-6.63064	3.956	3.956	3.956
12	-6.634308	3.952	3.952	3.952
13	-6.637545	3.948	3.948	3.948
14	-6.640342	3.944	3.944	3.944
15	-6.642689	3.94	3.94	3.94
16	-6.644576	3.936	3.936	3.936
17	-6.645993	3.932	3.932	3.932
18	-6.646929	3.928	3.928	3.928
19	-6.647374	3.924	3.924	3.924
20	-6.647437	3.92152	3.92152	3.92152
21	-6.647443	3.92095	3.92095	3.92095
22	-6.647443	3.920945	3.920945	3.920945
23	-6.647443	3.920945	3.920945	3.920945
24	-6.647443	3.920945	3.920945	3.920945
25	-6.647443	3.920945	3.920945	3.920945

Using the program, we found that the ground-state lattice constant is 3.920945 angstrom and a total potential energy of -6.647443 eV.

Ab) The next method we used to find the lattice constant was to manually adjust the lattice parameter in the file "lmp-in.1a-single" which also used the Lennard-Jones potential. Initially we started with a

lattice parameter of 3.92 as it was close to the relaxed lattice parameter we found in the first method. We then tested lattice parameters in intervals of 0.01 around 3.92 angstrom and recorded the total energy for each interval. Table 2 shows the lattice parameter that was plugged into our code and the resulting total energy. Figure 1 shows a graph of the crystal energy as a function of the lattice parameter and a fitted trendline and the corresponding equation.

Table 2: Lattice Constant Used and Resulting Energy from Results from lmp-in.1a-single

Lattice Constant (Angstrom)	Total Energy (eV)
4	-6.56442
3.99	-6.5833
3.98	-6.60009
3.97	-6.61454
3.96	-6.62655
3.95	-6.63598
3.94	-6.64268
3.93	-6.646521
3.92	-6.647428
3.91	-6.645501
3.9	-6.640205
3.89	-6.631357
3.88	-6.618766
3.87	-6.602231

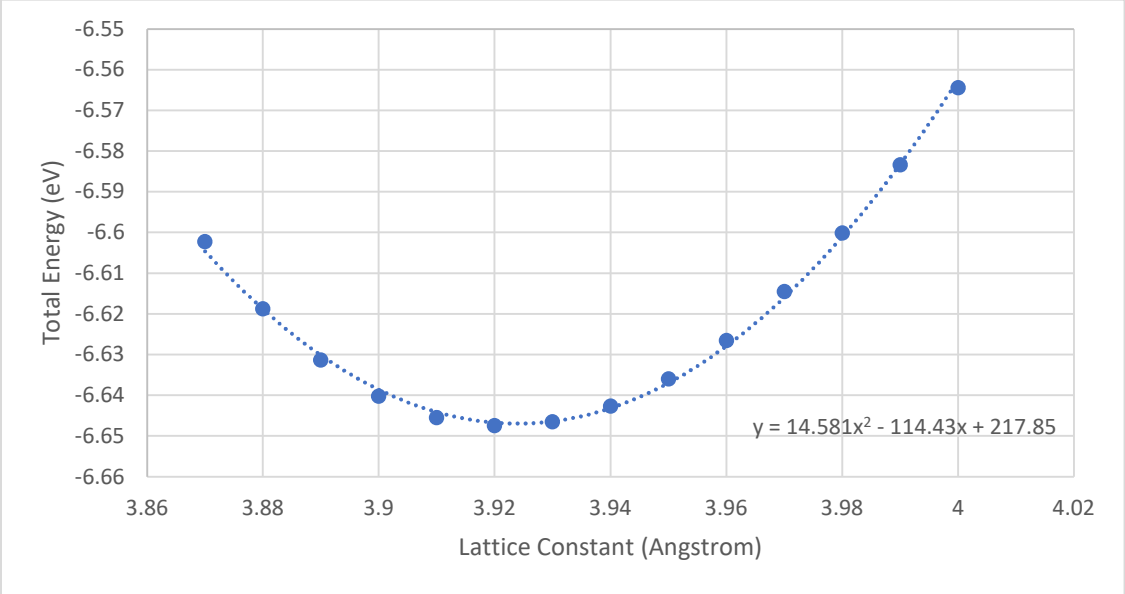

Figure 1: Total Energy as a Function of Lattice Parameter Using Lennard-Jones Potential

Using the fitted trendline equation we found the equilibrium lattice constant to be 3.92394 angstrom which correlated to a total energy of -6.65835 eV.

B) The final method we used to calculate the equilibrium lattice constant was to use the Embedded Atom Model (EAM) potential. We first ran the EAM input file with the built-in minimizer, "lmp-in.1b-relax", and used the PT-Adams1989.eam data file. We found that the equilibrium lattice constant was 3.9200001 angstrom and the total energy to be -23.07999 eV. We then used the EAM input file that did not include the built-in minimizer, ""lmp-in.1b-single", and manually adjusted the lattice parameter to create a graph of the total energy versus the lattice parameter in a similar way to the Lennard Jones potential calculation in part 1Ab. Table 3 shows the lattice parameter that was plugged into our EAM input file and the resulting total energy. Figure 2 shows a graph of the crystal energy as a function of the lattice parameter and a fitted trendline and the corresponding equation.

Table 3: Lattice Constant Used and Resulting Energy from Results from lmp-in.1b-single

Lattice Constant (angstrom)	Total Energy (eV)
4	-22.897
3.99	-22.938
3.98	-22.975
3.97	-23.006
3.96	-23.032
3.95	-23.053
3.94	-23.068
3.93	-23.077
3.92	-23.079
3.91	-23.077
3.9	-23.067
3.89	-23.051
3.88	-23.028
3.87	-22.998

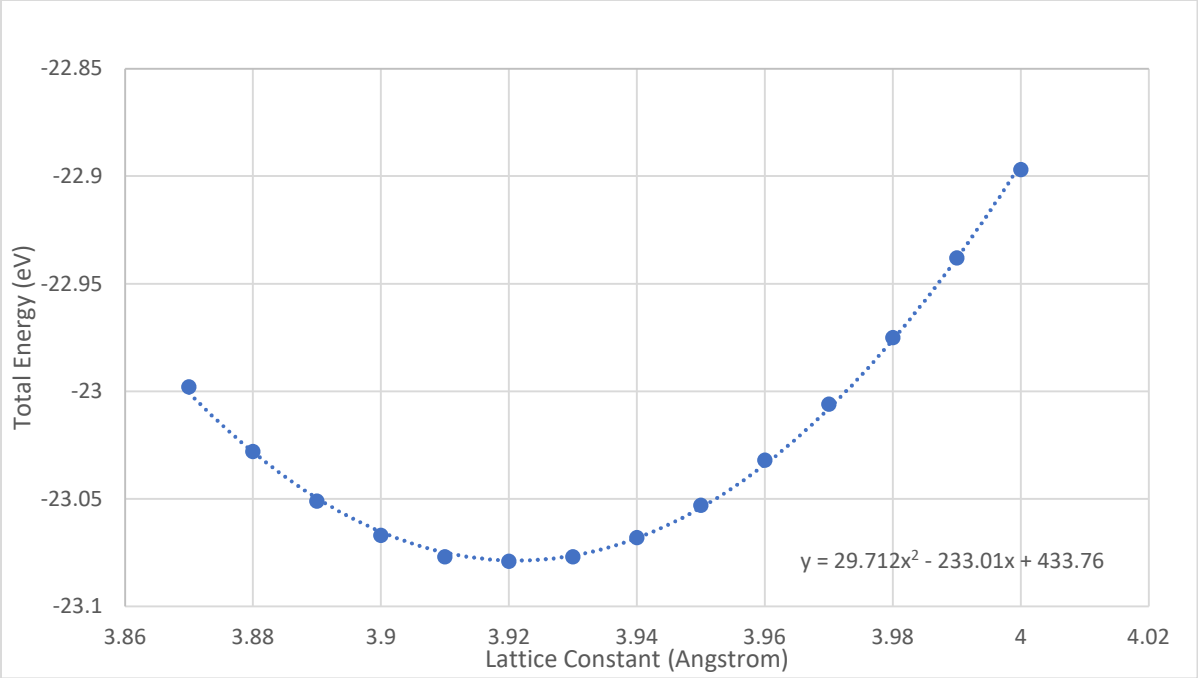

Figure 2: Total Energy as a Function of Lattice Parameter from EAM Potential

Using the fitted trendline equation we found the equilibrium lattice constant to be 3.921 angstrom which correlated to a total energy of -23.081 eV.

C) The lattice constants found using the Lennard-Jones and EAM potentials both agree well with the experimentally found lattice constant of 3.92 angstrom. This is to be expected as both potentials are fitted to experiments. However, the lattice energies found were very different. For Lennard-Jones potential we found an absolute lattice energy value of 6.647 eV and 6.658 eV while the EAM potential gave us 23.0799 and 23.081 eV. This is due to the different energy methods used and thus they will give different lattice energies. What is most important is that the energy values between structures within an energy method are similar which the Lennard-Jones and EAM are.

Problem 2:

To compute the vacancy energy formation, E_v we used the equation:

$$E_v = E_{N-1} - \frac{N-1}{N} E_{bulk}$$

Where E_{bulk} is the energy of the perfect bulk supercell and E_{N-1} is the energy of the defect cell, while N is the number of atoms in the supercell. We have to include the $\frac{N-1}{N}$ factor in order to compare the energy of the defective supercell to the perfect cell.

We also need to modify our code in order to correctly calculate E_{N-1}. The code "group vacancy id <=1" and "delete_atoms group vacancy" was added to our files which can be seen in Figure 5, 6, and 7

of Appendix A. This will allow us to calculate E_{N-1} as these lines of code will remove one atom from our supercell to create the defect cell.

A) We first want to calculate the vacancy formation energy by using the unrelaxed Lennard Jones potential with a lattice constant of 3.921. We created three different supercells of sizes 1x1x1, 3x3x3, and 5x5x5 in order to test for convergence which gave us the following vacancy energy formations:

1x1x1 super cell:

$$E_v = -3.544 - \frac{3}{4}(-6.647) = 1.441\ eV$$

3x3x3 super cell:

$$E_v = -176.157 - \frac{107}{108}(-179.481) = 1.662\ eV$$

5x5x5 super cell:

$$E_v = -827.607 - \frac{499}{500}(-830.930) = 1.661\ eV$$

We found the vacancy formation energy to converge to 1.662 eV. We also calculated the cohesive energy by using the equation below:

$$E_{cohesive} = E_{compound} - \sum E_{atom}$$

Where $E_{compound}$ is equal to E_{bulk} of the given supercell and E_{atom} is equal to the energy of a single atom. $E_{cohesive}$ was found to be 6.648 eV. The ratio of E_v to $E_{cohesive}$ was calculated to be 0.25. This matches the results of other FCC metals so it is expected.

B) The next method we used to calculate the vacancy formation energy is to relax the Lennard-Jones potential after the vacancy has been created. The relaxation started from a lattice parameter of 4 angstroms. Vacancy formation energy was calculated the same way as before and below are the results:

1x1x1 super cell:

$$E_v = -3.547 - \frac{3}{4}(-6.647) = 1.438\ eV$$

3x3x3 super cell:

$$E_v = -176.179 - \frac{107}{108}(-179.481) = 1.640\ eV$$

5x5x5 super cell:

$$E_v = -827.629 - \frac{499}{500}(-830.930) = 1.639\ eV$$

Using the relaxed Lennard-Jones potential we found that the vacancy energy formation converged to 1.640 eV. This is similar to the vacancy formation energy that was found using the unrelaxed method which was 1.662 eV. The ratio of E_v to $E_{cohesive}$ was calculated to be 0.247.

C) The third method we used to calculate the vacancy energy formation was to use the Embedded Atom Model potential. The set up was identical to the relaxed Lennard Jones potential but instead of using "lmp-in.1a-relax" we used "lmp-in.1b-relax" but still started with the lattice parameter set to 4 angstroms. This gave us the following results:

1x1x1 super cell:

$$E_v = -15.615 - \frac{3}{4}(-23.079) = 1.694\ eV$$

3x3x3 super cell:

$$E_v = -615.625 - \frac{107}{108}(-623.159) = 1.764\ eV$$

5x5x5 super cell:

$$E_v = -2877.442 - \frac{499}{500}(-2884.999) = 1.787\ eV$$

6x6x6 super cell:

$$E_v = -4977.720 - \frac{863}{864}(-4985.279) = 1.789\ eV$$

We found that the vacancy formation energy converges to 1.789 eV. The ratio of E_v to $E_{cohesive}$ was calculated to be 0.269.

D) The experimental vacancy energy formation was found to be between 1.6 and 1.77 eV. Our relaxed Lennard-Jones vacancy energy formation of 1.640 eV is within this range but our EAM vacancy

energy formation of 1.789 eV is just outside of it. Comparing this to problem 1, it seems Lennard Jones potential is more accurate than EAM potential for calculating vacancy energy formations which does not seem right as EAM should do better at simulating metals.

Problem 3:

Surface energy is calculated using equation seen below:

$$E_{surface} = \frac{1}{2A}(E_{slab} - \frac{N}{N_0}E_{bulk})$$

Where $E_{surface}$ is the surface energy, E_{slab} is the energy of the slab with vacuum, E_{bulk} is the energy of the bulk slab, and A is the surface area of the slab. N is the number of atoms in the slab with vacuum and N_0 is the number of atoms in the bulk slab. N and N_0 will be the same for this problem as no atoms are being removed. It is important that each slab does not see another slab so the vacuum between them must be large. It is also important that deep inside the slab the atoms are the same as the bulk slab. Both of these problems can be solved using large supercells with large vacuum layers. We decided to use 30 x 1 x 1 supercells to best test the convergence of the surface energy because this solves the aforementioned problems as well as being more computationally efficient compared to supercells that expand in the y and z directions. We do not need cells in the y or z directions since interatomic potentials do not require 3d periodicity.

The line "Change_box all x delta 0.0 2.0 units lattice" was added to our files that enabled us to build the slab model as it inserted a vacuum region using the parameters that it was told. This can be seen in Figure 8 and 9 of Appendix A.

A) For Lennard jones potential the following calculations were done using a lattice parameter of 3.92 angstroms and a unit cell of 30 x 1 x1:

Vacuum region of 1 lattice:

$$E_{surface} = \frac{1}{2(3.92 * 3.92)}\left(-196.752 - \frac{120}{120}(-199.423)\right) = .0869\ \frac{eV}{Å^2}$$

Vacuum region of 1.5 lattice:

$$E_{surface} = \frac{1}{2(3.92 * 3.92)}\left(-196.692 - \frac{120}{120}(-199.423)\right) = .089\ \frac{eV}{Å^2}$$

Vacuum region of 2 lattice:

$$E_{surface} = \frac{1}{2(3.92 * 3.92)}\left(-196.685 - \frac{120}{120}(-199.423)\right) = .089\ \frac{eV}{Å^2}$$

Vacuum region of 5 lattice:

$$E_{surface} = \frac{1}{2(3.92 * 3.92)}\left(-196.685 - \frac{120}{120}(-199.423)\right) = .089\ \frac{eV}{Å^2}$$

B) We used the same method and parameters to calculate surface energy with the EAM potential:

$$E_{surface} = \frac{1}{2(3.92 * 3.92)}\left(-689.116 - \frac{120}{120}(-692.399)\right) = .107\ \frac{eV}{Å^2}$$

Vacuum region of 1.5 lattice:

$$E_{surface} = \frac{1}{2(3.92 * 3.92)}\left(-688.930 - \frac{120}{120}(-692.399)\right) = .113\ \frac{eV}{Å^2}$$

Vacuum region of 2 lattice:

$$E_{surface} = \frac{1}{2(3.92 * 3.92)}\left(-688.930 - \frac{120}{120}(-692.399)\right) = .113\ \frac{eV}{Å^2}$$

Vacuum region of 5 lattice:

$$E_{surface} = \frac{1}{2(3.92 * 3.92)}\left(- - 688.930 - \frac{120}{120}(-692.399)\right) = .113\ \frac{eV}{Å^2}$$

We found the surface energy of (1 0 0) FCC platinum to be 0.089 $\frac{eV}{Å^2}$ using Lennard-Jones potential and .113 $\frac{eV}{Å^2}$ using EAM potential.

Problem 4:

The Lennard Jones potential is most suitable for materials such as noble gases or diatomic molecules. Lennard Jones potentials are also useful in modelling/simulating interactions between simple atoms or molecules and non-directed interactions. EAM potentials are best used for problems that need to model metallic bonding/ metallic systems. However, Lennard Jones and EAM potentials are not appropriate to use for covalent bonded atoms/molecules or to figure out the angle dependance of a molecule which is useful for figuring out the energy difference in organic molecules.

Problem 5:

To minimize the Lennard-Jones potential we must take the derivative of $V_{LJ}(r)$ which will give us:

$$\frac{dV_{LJ}(r)}{dr} = 0 = \frac{-12\sigma^{12}}{r^{13}} + \frac{6\sigma^{6}}{r^{7}}$$

$$\frac{12\sigma^{12}}{r^{13}} = \frac{6\sigma^{6}}{r^{7}}$$

$$1 = \frac{2\sigma^{6}}{r^{6}}$$

$$r = \sigma\sqrt[6]{2}$$

Plugging in σ= 2.540 we get r=2.851 angstrom. This is different than the equilibrium lattice constant of 3.92 we found in problem 1. However, this is because the lattice constant found in problem 1 is for the length of the unit cell while the 2.851 angstroms from the hand calculation describes the distance between the nearest atomic neighbors. The length of the unit cell and the distance to the nearest neighbor can be related if we divide the length of the unit cell by a factor of $\sqrt{2}$. This gives us a distance to nearest neighbor for the Lennard-Jones potential of 2.772 angstrom. There is still a discrepancy between the two values which is due to the hand calculated value only factoring in two atoms while the Lennard-Jones value is for a periodic crystal that has more interactions between atoms and thus brings the atoms closer together.

Contributors: N/A I worked alone for this project

Appendix A:

Table A: Provided Files from Instructor

File	Description	Comment
lmp-in.1a-single	LAMMPS input file for a single point calculation of FCC Pt using a Lennard-Jones potential	
lmp-in.1a-relax	LAMMPS input file for geometry optimizations (relaxations) using a Lennard-Jones potential	
lmp-in.1b-single	LAMMPS input file for a single point calculation of FCC Pt using an EAM potential	EAM potential file required
lmp-in.1b-relax	LAMMPS input file for geometry optimizations (relaxations) using an EAM potential	EAM potential file required
Pt-Adams1989.eam	EAM potential for Pt. This potential was published in Adams et al., *J. Mater. Res.* **4**, 102-112 (1989) and can be obtained from http://www.ctcms.nist.gov/potentials	

Figure 1: Code for lmp-in.1a-relax, Lennard-Jones potential with relaxation (problem 1 Aa)

```
# ------------------------------------------------------------------------
# Columbia University - CHEN E4880 - Project 1
# LAMMPS input file for problem 1a
# Geometry relaxation of FCC Pt using a Lennard-Jones potential
# ------------------------------------------------------------------------

# Initial set-up
clear
units metal
dimension 3
boundary p p p
atom_style atomic

# Create atoms
lattice      fcc 4.0 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       simulation_box block 0 1 0 1 0 1 units lattice
create_box   1 simulation_box
create_atoms 1 box

# Supercell
replicate    1 1 1

# Atomic mass (in amu)
mass 1 195.084

# Lennard-Jones potential
#   epsilon = 0.200 eV
#   sigma   = 2.540 Ang
pair_style lj/cut 10.0
pair_coeff 1 1 0.200 2.540
pair_modify shift yes

# When to write out the optimized structure
dump atom all custom 50 dump*.cfg id type x y z

# Structure optimization
fix 1 all box/relax iso 0.0 vmax 0.001
thermo 1
thermo_style custom step pe lx ly lz
minimize 1e-15 1e-15 5000 10000

# Write out total energy
variable potential_energy equal "pe"
print "Total energy (eV) = ${potential_energy};"
```

Figure 2: Code for lmp-in.1a-single, Lennard-Jones potential with no relaxation (problem 1 Ab)

```
# ----------------------------------------------------------------------
# Columbia University - CHEN E4880 - Project 1
# LAMMPS input file for problem 1a
# Single point calculation for FCC Pt using a Lennard-Jones potential
# ----------------------------------------------------------------------

# Initial set-up
clear
units metal
dimension 3
boundary p p p
atom_style atomic

# Create FCC Au structure
lattice      fcc 3.92 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       simulation_box block 0.0 1.0 0.0 1.0 0.0 1.0 units lattice
create_box   1 simulation_box
create_atoms 1 box

# Create supercell
replicate 1 1 1

# Atomic mass (in amu)
mass 1 195.084

# Lennard-Jones potential
#   epsilon = 0.200 eV
#   sigma   = 2.540 Ang
pair_style lj/cut 10.0
pair_coeff 1 1 0.200 2.540
pair_modify shift yes

# Evaluate the energy of the input structure
fix 1 all nve
thermo_style custom step pe lx ly lz
run 0

# Write out total energy
variable potential_energy equal "pe"
print "Total energy (eV) = ${potential_energy};"
```

Figure 3: Code for lmp-in.1b-single, EAM potential with no relaxation (problem 1B)

```
# ----------------------------------------------------------------------
# Columbia University - CHEN E4880 - Project 1
# LAMMPS input file for problem 1b
# Single point calculation for FCC Pt using an EAM potential
# ----------------------------------------------------------------------

# Initial set-up
clear
units metal
dimension 3
boundary p p p
atom_style atomic

# Create atoms
lattice      fcc 3.92 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       simulation_box block 0 1 0 1 0 1 units lattice
create_box   1 simulation_box
create_atoms 1 box

# Create supercell
replicate 1 1 1


# Atomic mass (in amu)
mass 1 195.084

# EAM potential
#   required file:
pair_style eam
pair_coeff * * Pt-Adams1989.eam

# When to write out the optimized structure
dump atom all custom 50 dump*.cfg id type x y z

# Evaluate the energy of the input structure
fix 1 all nve
thermo_style custom step pe lx ly lz
run 0

# Output
variable potential_energy equal "pe"
print "Total energy (eV) = ${potential_energy};"
```

Figure 4: Code for lmp-in.1b-relax, EAM potential with relaxation (problem 1B)

```
# ------------------------------------------------------------------------
# Columbia University - CHEN E4880 - Project 1
# LAMMPS input file for problem 1b
# Geometry relaxation of FCC Pt using an EAM potential
# ------------------------------------------------------------------------

# Initial set-up
clear
units metal
dimension 3
boundary p p p
atom_style atomic

# Create atoms
lattice      fcc 4.0 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       simulation_box block 0 1 0 1 0 1 units lattice
create_box   1 simulation_box
create_atoms 1 box

# Create supercell
replicate    1 1 1

# Atomic mass (in amu)
mass 1 195.084

# EAM potential
#   required file:
pair_style eam
pair_coeff * * Pt-Adams1989.eam

# When to write out the optimized structure
dump atom all custom 50 dump*.cfg id type x y z

# Structure optimization
fix 1 all box/relax iso 0.0 vmax 0.001
thermo 1
thermo_style custom step pe lx ly lz
minimize 1e-8 1e-8 5000 10000

# Output
variable potential_energy equal "pe"
print "Total energy (eV) = ${potential_energy};"
```

Figure 5: Lennard-Jones potential with no relaxation and atom vacancy (Problem 2a)

```
# ----------------------------------------------------------------------
# Columbia University - CHEN E4880 - Project 1
# LAMMPS input file for problem 2a
# Single point calculation for FCC Pt using a Lennard-Jones potential
# ----------------------------------------------------------------------

# Initial set-up
clear
units metal
dimension 3
boundary p p p
atom_style atomic

# Create FCC Au structure
lattice      fcc 3.921 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       simulation_box block 0.0 1.0 0.0 1.0 0.0 1.0 units lattice
create_box   1 simulation_box
create_atoms 1 box

# Create supercell
replicate 5 5 5

group vacancy id <= 1
delete_atoms group vacancy

# Atomic mass (in amu)
mass 1 195.084

# Lennard-Jones potential
#   epsilon = 0.200 eV
#   sigma   = 2.540 Ang
pair_style lj/cut 10.0
pair_coeff 1 1 0.200 2.540
pair_modify shift yes

# Evaluate the energy of the input structure
fix 1 all nve
thermo_style custom step pe lx ly lz
run 0

# Write out total energy
variable potential_energy equal "pe"
print "Total energy (eV) = ${potential_energy};"
```

Figure 6: Lennard-Jones potential with relaxation and atom vacancy (Problem 2b)

```
# LAMMPS input file for problem 2b
# Geometry relaxation of FCC Pt using a Lennard-Jones potential
# ----------------------------------------------------------------------

# Initial set-up
clear
units metal
dimension 3
boundary p p p
atom_style atomic

# Create atoms
lattice      fcc 4 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       simulation_box block 0 1 0 1 0 1 units lattice
create_box   1 simulation_box
create_atoms 1 box

# Supercell
replicate    3 3 3

group vacancy id <= 1
delete_atoms group vacancy

# Atomic mass (in amu)
mass 1 195.084

# Lennard-Jones potential
#   epsilon = 0.200 eV
#   sigma   = 2.540 Ang
pair_style lj/cut 10.0
pair_coeff 1 1 0.200 2.540
pair_modify shift yes

# When to write out the optimized structure
dump atom all custom 50 dump*.cfg id type x y z

# Structure optimization
fix 1 all box/relax iso 0.0 vmax 0.001
thermo 1
thermo_style custom step pe lx ly lz
minimize 1e-15 1e-15 5000 10000

# Write out total energy
variable potential_energy equal "pe"
print "Total energy (eV) = ${potential_energy};"
```

Figure 7: EAM potential with relaxation and atom vacancy (Problem 2c)

```
# ----------------------------------------------------------------------
# Columbia University - CHEN E4880 - Project 1
# LAMMPS input file for problem 2c
# Geometry relaxation of FCC Pt using an EAM potential
# ----------------------------------------------------------------------

# Initial set-up
clear
units metal
dimension 3
boundary p p p
atom_style atomic

# Create atoms
lattice      fcc 4.0 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       simulation_box block 0 1 0 1 0 1 units lattice
create_box   1 simulation_box
create_atoms 1 box

# Create supercell
replicate    3 3 3

group vacancy id <= 1
delete_atoms group vacancy

# Atomic mass (in amu)
mass 1 195.084

# EAM potential
#   required file:
pair_style eam
pair_coeff * * Pt-Adams1989.eam

# When to write out the optimized structure
dump atom all custom 50 dump*.cfg id type x y z

# Structure optimization
fix 1 all box/relax iso 0.0 vmax 0.001
thermo 1
thermo_style custom step pe lx ly lz
minimize 1e-8 1e-8 5000 10000

# Output
variable potential_energy equal "pe"
print "Total energy (eV) = ${potential_energy};"
```

Figure 8: Lennard-Jones potential with vacuum inserted (Problem 3a)

```
# ------------------------------------------------------------------------
# Columbia University - CHEN E4880 - Project 1
# LAMMPS input file for problem 3a
# Single point calculation for FCC Pt using a Lennard-Jones potential
# ------------------------------------------------------------------------

# Initial set-up
clear
units metal
dimension 3
boundary p p p
atom_style atomic

# Create FCC Au structure
lattice      fcc 3.921 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       simulation_box block 0.0 1.0 0.0 1.0 0.0 1.0 units lattice
create_box   1 simulation_box
create_atoms 1 box

# Create supercell
replicate 30 1 1

change boc all x delta 0.0 2.0 units lattice

# Atomic mass (in amu)
mass 1 195.084

# Lennard-Jones potential
#   epsilon = 0.200 eV
#   sigma   = 2.540 Ang
pair_style lj/cut 10.0
pair_coeff 1 1 0.200 2.540
pair_modify shift yes

# Evaluate the energy of the input structure
fix 1 all nve
thermo_style custom step pe lx ly lz
run 0

# Write out total energy
variable potential_energy equal "pe"
print "Total energy (eV) = ${potential_energy};"
```

Figure 9: EAM potential with vacuum inserted (Problem 3b)

```
# ----------------------------------------------------------------------
# Columbia University - CHEN E4880 - Project 1
# LAMMPS input file for problem 3b
# Single point calculation for FCC Pt using an EAM potential
# ----------------------------------------------------------------------

# Initial set-up
clear
units metal
dimension 3
boundary p p p
atom_style atomic

# Create atoms
lattice      fcc 3.921 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       simulation_box block 0 1 0 1 0 1 units lattice
create_box   1 simulation_box
create_atoms 1 box

# Create supercell
replicate 30 1 1

change_box all x delta 0.0 2.0 units lattice


# Atomic mass (in amu)
mass 1 195.084

# EAM potential
#   required file:
pair_style eam
pair_coeff * * Pt-Adams1989.eam

# When to write out the optimized structure
dump atom all custom 50 dump*.cfg id type x y z

# Evaluate the energy of the input structure
fix 1 all nve
thermo_style custom step pe lx ly lz
run 0

# Output
variable potential_energy equal "pe"
print "Total energy (eV) = ${potential_energy};"
```