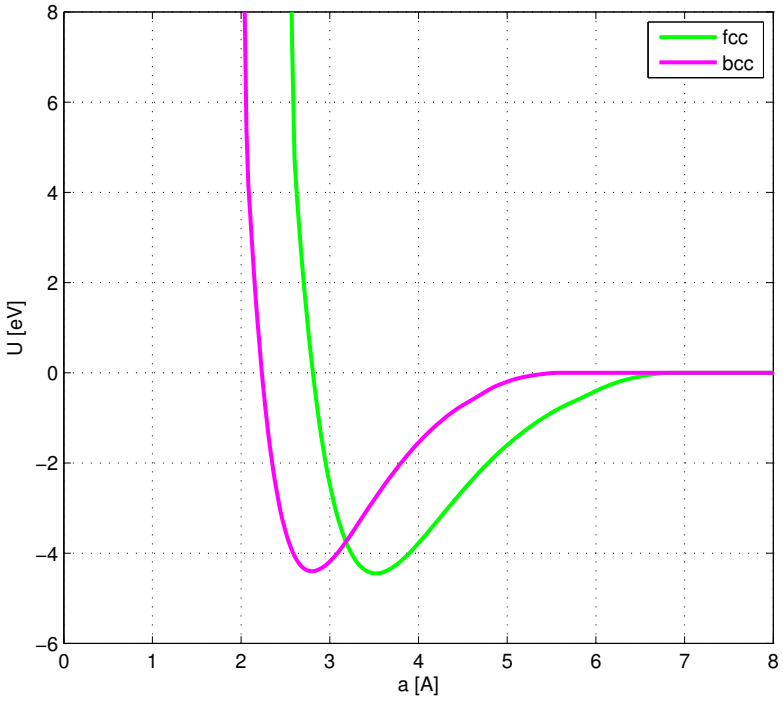
Report I
Atomistic modeling

This report shows the mechanical properties of Nickel, obtained from Molecular Dynamics computations. The objectives of the analysis are the stability of the crystalline structure, the density, the linear thermal expansion coefficient and the elastic parameters of Nickel.

The numerical simulations were performed using LAMMPS software. In the *Appendix* it is possible to find the script and some input files that have been used.

1 Lattice constant and cohesive energy

The first simulation concerns the lattice constant and the cohesive energy for *fcc* and *bcc* Ni structure at $T = 0\,K$. A three-dimensional box with 5 unit cells per side is created, starting with an initial value of lattice constant a_0. Using the Embedded Atom Model potential, the software expands the box and computes the cohesive energy for the particular value of the distance between unit cells.



The previous graph shows the potential as a function of the distance. The output value is normalized to the number of atoms (500 for the *fcc* box, 250 for the *bcc*) and the length of the box is divided by 5, the number elementary units along the side (*Appendix b*).

The minimum value of the potential for each structure is:

fcc	*bcc*
$U_0 = -4.4492\, eV$	$U_0 = -4.4016\, eV$
$a = 3.5064\,$ Å	$a = 2.8052\,$ Å

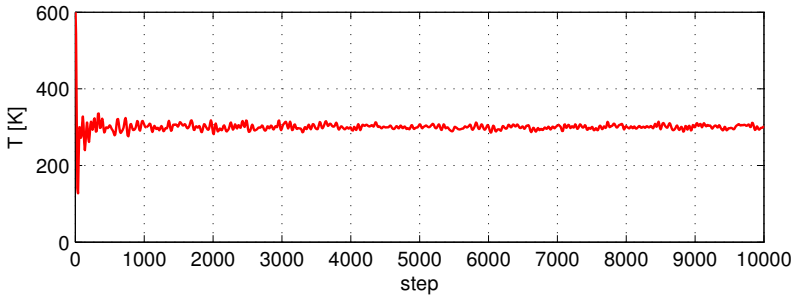
As it is possible to see, the potential for *fcc* structure is lower that *bcc*; this means that the face-centered cubic structure is more stable. The value of the lattice constant ($a = 3.5064\,$ Å) will be used in the next simulations.

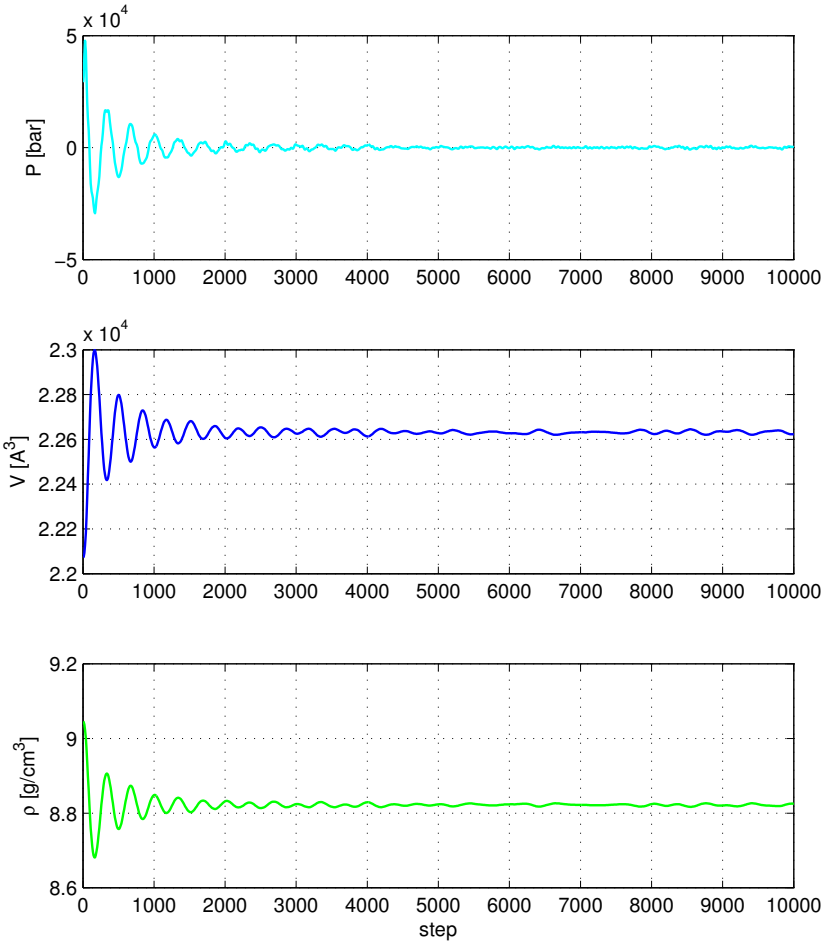
2 Density and linear thermal expansion coefficient

A different type of analysis is performed to obtain the density of Nickel. A box is created with a *fcc* structure and the lattice constant found at the previous stage. In order to ensure stability of the solution, the unit cells per side are 8. Then the potential is set up according to the EAM input file. After the minimization of the total energy to optimize the structure, it is ready for the proper computation.

With the appropriate arguments of the command *fix*, it is possible to execute a *NPT simulation*; first a velocity value is assigned to the atoms, setting the initial temperature to $T_0 = 600\, K$. Then the isothermal-isobaric simulation is launched, at a constant temperature of $T = 300\, K$ and a pressure of $P = 1\, atm$; the number of step is set to 10000. The requested outputs are the temperature, the pressure, the volume and the density.

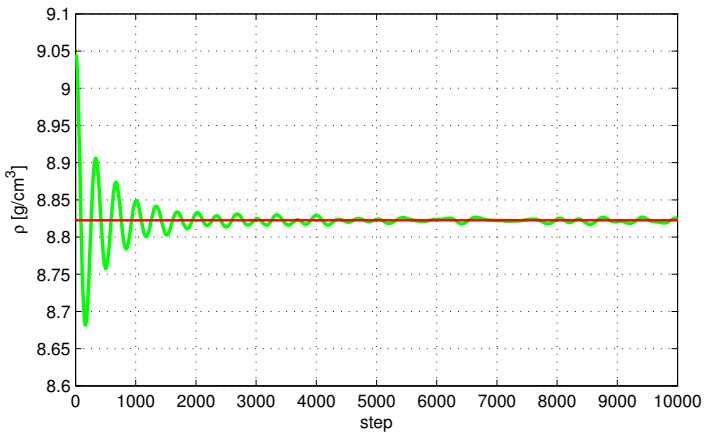
In the following the output variables at every time-step are presented; as can be seen from these figures, with an accurate choice of dumping parameters, the solution can be considered stable:



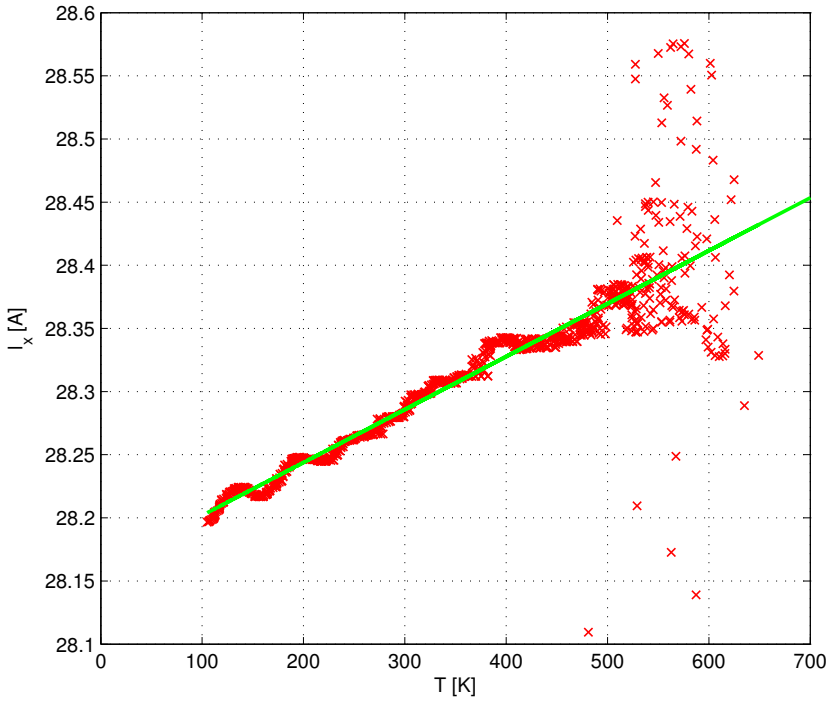


The average of the output data can be reasonably assumed to be a good estimation of the real value; for the density, the value found is

$$\rho = 8.8225\, g/cm^3$$



To find the linear thermal expansion coefficient a similar procedure to the previous is adopted. In this case the temperature is not constant, but it decreases from $T_i = 600\,K$ to $T_f = 100\,K$ (see *Appendix c*). The following graph shows the length of one dimension of the box versus the temperature:



To describe the trend of the data, the linear least square method has been used (the scattered data at the starting values of temperature have not been considered). It is possible to determine the thermal expansion form the slope of the line. As a matter of fact the LTE coefficient is:

$$\alpha = \frac{1}{L}\frac{dL}{dT} = 15.074 \cdot 10^{-6}\,K^{-1}$$

3 Stiffness tensor and mechanical parameters

LAMMPS software includes some example files, like the *ELASTIC* package; this is suitable for the calculation of the elastic constants. In the *Appendix d* and *Appendix e* there are two files that have been edited from those provided, for the atoms configuration and the potential respectively. It is necessary to set the *fcc* structure for nickel and the EAM potential must be given as input. The simulation returns the stiffness tensor components:

$$\begin{aligned} C_{11} = C_{22} = C_{33} &= 233.273\,GPa \\ C_{12} = C_{13} = C_{23} &= 154.287\,GPa \\ C_{44} = C_{55} = C_{66} &= 127.637\,GPa \end{aligned}$$

The other coefficients can be considered zero. From these results it is now possible to calculate the mechanical parameters of polycristalline Ni. For this purpose the Kröner model is adopted; the bulk modulus is

$$\kappa = \frac{1}{3}(c_{11} + 2c_{12}) = 180.61\, GPa$$

To calculate the shear modulus we need these two constant:

$$\mu_1 = \frac{1}{2}(c_{11} - c_{12}) = 39.49\, GPa$$

$$\mu_2 = c_{44} = 127.63\, GPa$$

Solving the following expression, it is possible to find the value of G:

$$G^3 + \gamma_1 G^2 + \gamma_2 G + \gamma_3 = 0$$

where the three constant are

$$\gamma_1 = \frac{9\kappa + 4\mu_1}{8} = 222.94$$

$$\gamma_2 = -\mu_2 \frac{3\kappa + 12\mu_1}{8} = -16206$$

$$\gamma_3 = -\frac{3\kappa\mu_1\mu_2}{4} = -6.828e5$$

The only real solution of the previous equation is

$$G = 81.03\, GPa$$

Finally we cand find the Young's modulus and Poisson's ratio

$$E = -\frac{9\kappa G}{(3\kappa + G)} = 211.48\, GPa$$

$$\nu = \frac{3\kappa - 2G}{2(3\kappa + G)} = 0.3049$$

4 Elastic constants of nano-crystalline Ni

Even in this case the procedure is similar to the previous point, but the atoms location is given by an input file that contains the structure of a nano-crystalline Ni model (equilibrated at $T = 10\, K$ and quenched after $10\, ps$ thermal annealing at $T = 1000\, K$). The minimization parameters are set in order to ensure the accuracy of the solution. The results are

$$\begin{aligned} C_{11} &= 243.46\, GPa \\ C_{22} &= 241.05\, GPa \\ C_{33} &= 235.82\, GPa \end{aligned}$$

$$
\begin{aligned}
C_{12} &= 136.13\,GPa \\
C_{13} &= 140.18\,GPa \\
C_{23} &= 142.19\,GPa
\end{aligned}
$$

$$
\begin{aligned}
C_{44} &= 46.747\,GPa \\
C_{55} &= 46.870\,GPa \\
C_{66} &= 46.533\,GPa
\end{aligned}
$$

The triplets are not exactly equal and the other components of the tensor are small but not zero; it is possible to make an approximation and then consider the solid as cubic system. Hence these data are averaged and reduced to the following values

$$
\begin{aligned}
\overline{C}_{11} &= 240.11\,GPa \\
\overline{C}_{12} &= 139.50\,GPa \\
\overline{C}_{44} &= 46.72\,GPa
\end{aligned}
$$

To check if this model can be regarded as a continuum the anisotropic parameter is calculated; if A is equal to 1, then the system is elastically equivalent to an isotropic continuum:

$$
A = \frac{2\overline{C}_{44}}{\overline{C}_{11} - \overline{C}_{12}} = 0.9287
$$

Therefore this nano-crystalline system can be regarded approximately as a continuum, if a sufficiently big scale is considered.

Appendix

a) Shell script

```
#!/bin/bash
#
# REPORT I - ATOMISTIC MODELING - Nanomechanics
# Shell script
#
# Damiano Milani
#

#source files path
source_path="/home/dami/Dropbox/courses/nanomechanics/reports/report1"
#LAMMPS path
lammps_path="/home/dami/.lammps/src/lmp_openmpi"


clear
echo -e "NANOMECHANICS - REPORT I \nATOMISTIC MODELING
Damiano Milani\n\n
Choose the task:
1) Lattice constant and cohesive energy, for fcc and bcc Ni T=0K
2) Density and linear thermal expansion coefficient, fcc Ni T=300K P=1atm
3) Elastic constants, fcc Ni
4) Elastic constants, nano-crystalline Ni
5) Exit\n"
read task;


case $task in
      1)
      ## 1 Lattice constant and cohesive energy
      clear
      echo "Task 1 - lattice constant, cohesive energy"
      echo "running..."
      # FCC
      # goto source file path
      cd $source_path/1
      # run lammps
      mpirun -np 2 $lammps_path < in_1fcc.ex > out_1fcc.ex
      #visual output
      less out_1fcc.ex
      grep -A1 Lx out_1fcc.ex | grep '[0-9]' > data_1fcc
      #plot
      gnuplot -p -e "plot 'data_1fcc"

      # BCC
      mpirun -np 2 $lammps_path < in_1bcc.ex > out_1bcc.ex
      less out_1bcc.ex
      grep -A1 Lx out_1bcc.ex | grep '[0-9]' > data_1bcc
      #plot
      gnuplot -p -e "plot 'data_1bcc"
      echo "completed!"
      ;;


      2)
      ## 2 Density and linear thermal expansion coeff (fcc T=300 P=1)
      clear
      echo "Task 2 - Density and linear thermal expansion coefficient"
      echo "running..."
      # goto source file path
      cd $source_path/2
      # 2.1 Density
      mpirun -np 2 $lammps_path < in_2rho.ex > out_2rho.ex
      less out_2rho.ex
      grep -A1001 Step out_2rho.ex | grep '[0-9]' | tail --lines=1001 > data_2rho
```

```
    # 2.2 Linear thermal expansione coeff
    mpirun -np 2 $lammps_path < in_2lte.ex > out_2lte.ex
    less out_2lte.ex
    grep -A1001 Step out_2lte.ex | grep '[0-9]' | tail --lines=1001 > data_2lte
    echo "completed!"
    ;;


    3)
    ## 3 Elastic constants, fcc Ni; mechanical parameters, poly Ni
    clear
    echo "Task 3 - Elastic constants, fcc Ni; mechanical parameters, poly Ni"
    echo "running..."
    cd $source_path/3
    mpirun -np 2 $lammps_path < in_3el.ex > out_3el.ex
    less out_3el.ex
    tail -n 21 out_3el.ex > data_3el
    echo "completed!"
    ;;


    4)
    ## 4 Elastic constants, fcc Ni; mechanical parameters, poly Ni
    clear
    echo "Task 4 - Elastic constants, nano-crystalline Ni"
    echo "running..."
    cd $source_path/4
    mpirun -np 2 $lammps_path < in_4nan.ex > out_4nan.ex
    less out_4nan.ex
    tail -n 21 out_4nan.ex > data_4nan
    echo "completed!"
    ;;


    5) exit;;
esac;

read
```

b) Cohesive energy, *fcc* Ni

```
# in_1fcc.ex
#
# Lattice constant and cohesive energy, for fcc Ni
#

units metal
atom_style atomic
boundary p p p

variable m        equal 58.6934
variable a0       equal 2.5

print "a0      = ${a0}"
print "mass    = ${m}"

lattice fcc ${a0}
region BOX block 0 5 0 5 0 5
create_box 1 BOX
create_atoms 1 box

mass 1 $m
```

```
pair_style eam
pair_coeff * * Ni_u3.eam

thermo_style custom lx pe

variable i loop 150
label loop
  run 0
  displace_box all x scale 1.01
  displace_box all y scale 1.01
  displace_box all z scale 1.01
next i
jump in_1fcc.ex loop
```

c) Linear thermal expansion coefficient

```
# in_2lte.ex
#     linear expansion coefficient
#     Ni fcc T=300K P=1atm
#

# system setup
units metal
boundary p p p
atom_style atomic

# creat fcc box
variable m        equal 58.6934
variable a0       equal 3.5064

lattice fcc ${a0}
region BOX block 0 8 0 8 0 8
create_box 1 BOX
create_atoms 1 box

# set up the EAM potential
pair_style eam
pair_coeff * * Ni_u3.eam

# variables definition
variable NA  equal 6.02214179e23                      # Avogadro constant
variable rho equal mass(all)/${NA}/(vol*1.0e-24)      # density
variable T0   equal 1200.0                            # creation temperature
variable T1   equal 600.0                             # initial temperature
variable T2   equal 100.0                             # final temperature

# set thermodynamical parameters for output
thermo_style custom step temp lx ly lz vol v_rho
thermo 10

# optimize the structure by minimizing the total energy
minimize 0. 0. 1000 10000

# set a dump file that includes all the trajectry of atoms
dump 1 all atom 100 dump.ex

# set the temperature, and run 10000 steps of NPT simulation
velocity all create ${T0} 3141592
fix 1 all npt temp ${T1} ${T2} 0.1 aniso 1.01325 1.01325 2.0
timestep 0.001
run 10000
```

d) Configuration for elastic parameters

```
## init.mod

# Define the finite deformation size. Try several values of this
# variable to verify that results do not depend on it.
variable up equal 1.0e-6

# metal units, elastic constants in GPa
units          metal
variable cfac equal 1.0e-4
variable cunits string GPa

# Define minimization parameters
variable etol equal 0.0
variable ftol equal 1.0e-10
variable maxiter equal 100
variable maxeval equal 1000
variable dmax equal 1.0e-3

# generate the box and atom positions using a fcc lattice
variable a equal 3.5064

boundary  p p p
lattice         fcc $a
region         box prism 0 2.0 0 3.0 0 4.0 0.0 0.0 0.0
create_box     1 box
create_atoms   1 box

# Need to set mass to something, just to satisfy LAMMPS
mass 1 1.0e-20
```

e) Potential for the elastic constants

```
## potential.mod

# Choose potential
pair_style     eam
pair_coeff * * Ni_u3.eam

# Setup neighbor style
neighbor 1.0 nsq
neigh_modify once no every 1 delay 0 check yes

# Setup minimization style
min_style      cg
min_modify          dmax ${dmax} line quadratic

# Setup output
thermo         1
thermo_style custom step temp pe press pxx pyy pzz pxy pxz pyz lx ly lz vol
thermo_modify norm no
```