# Au Nanowires

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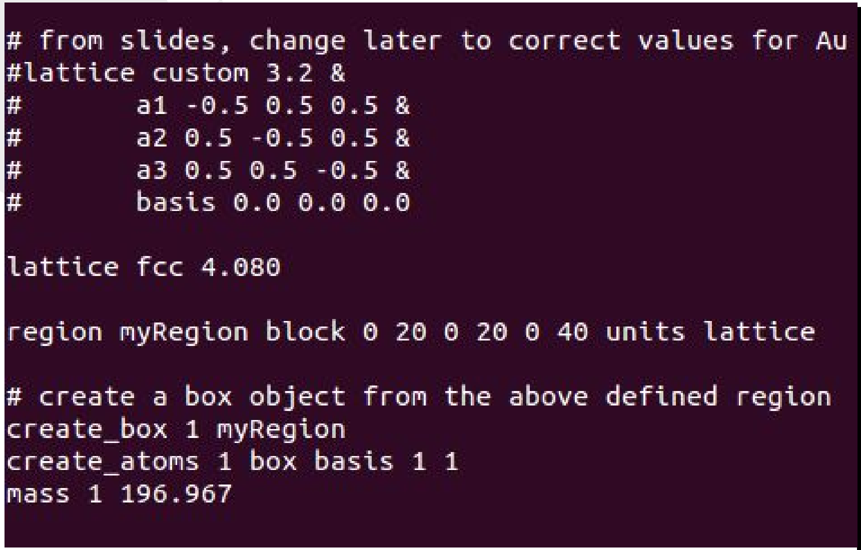
## Define Project

Project option 1

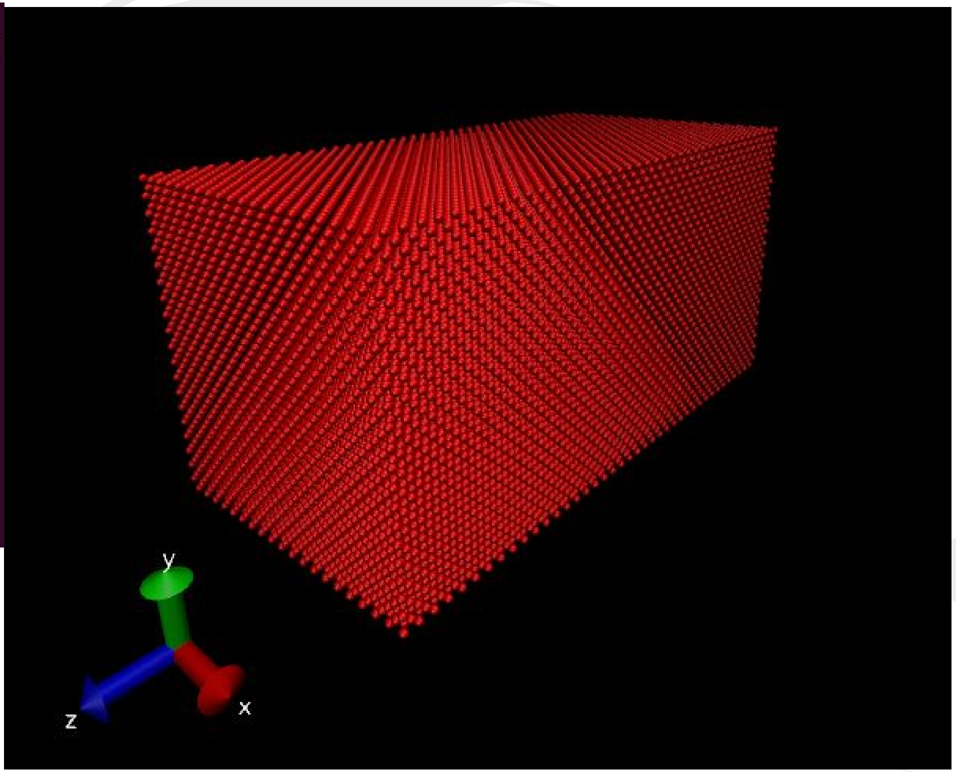
Create a bulk gold model, carve out nanowires from the bulk along different crystal directions (e.g. <111>, <100>, <110> etc.

1. Compare the energetics of these nanowires after energy minimization.
2. Test the elastic properties of these nanowires and try to understand the phenomenon.

# Creating the Bulk

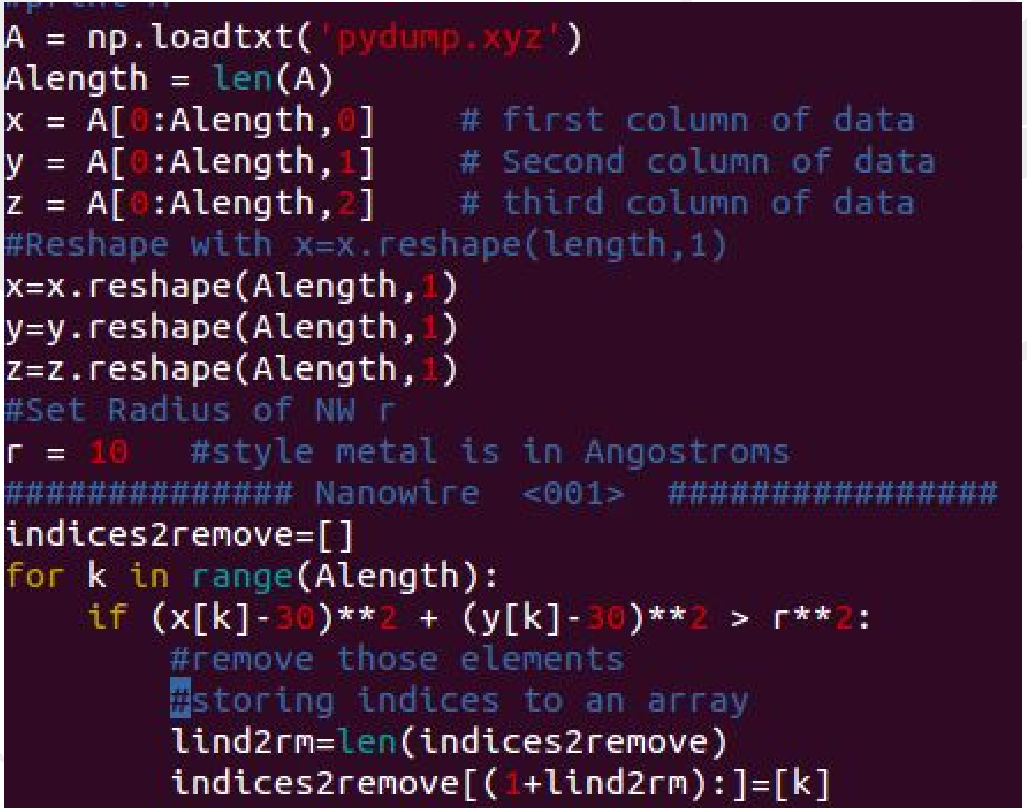


```
# from slides, change later to correct values for Au
#lattice custom 3.2 &
#       a1 -0.5 0.5 0.5 &
#       a2 0.5 -0.5 0.5 &
#       a3 0.5 0.5 -0.5 &
#       basis 0.0 0.0 0.0

lattice fcc 4.080

region myRegion block 0 20 0 20 0 40 units lattice

# create a box object from the above defined region
create_box 1 myRegion
create_atoms 1 box basis 1 1
mass 1 196.967
```

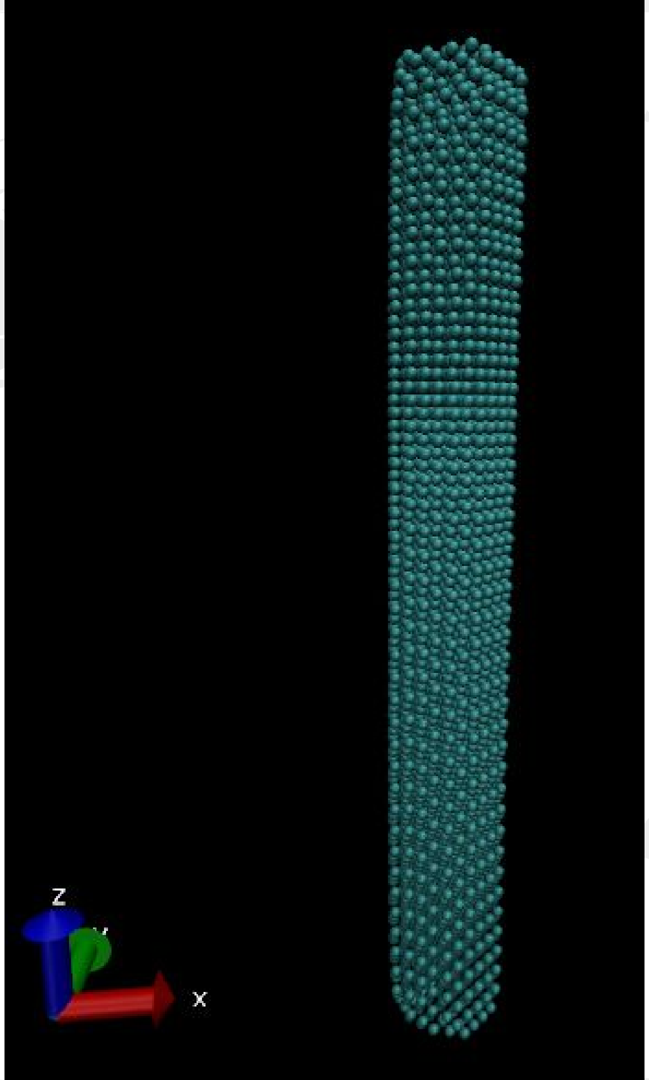


- Created brick of 64,000 atoms
- Energy -251,520eV

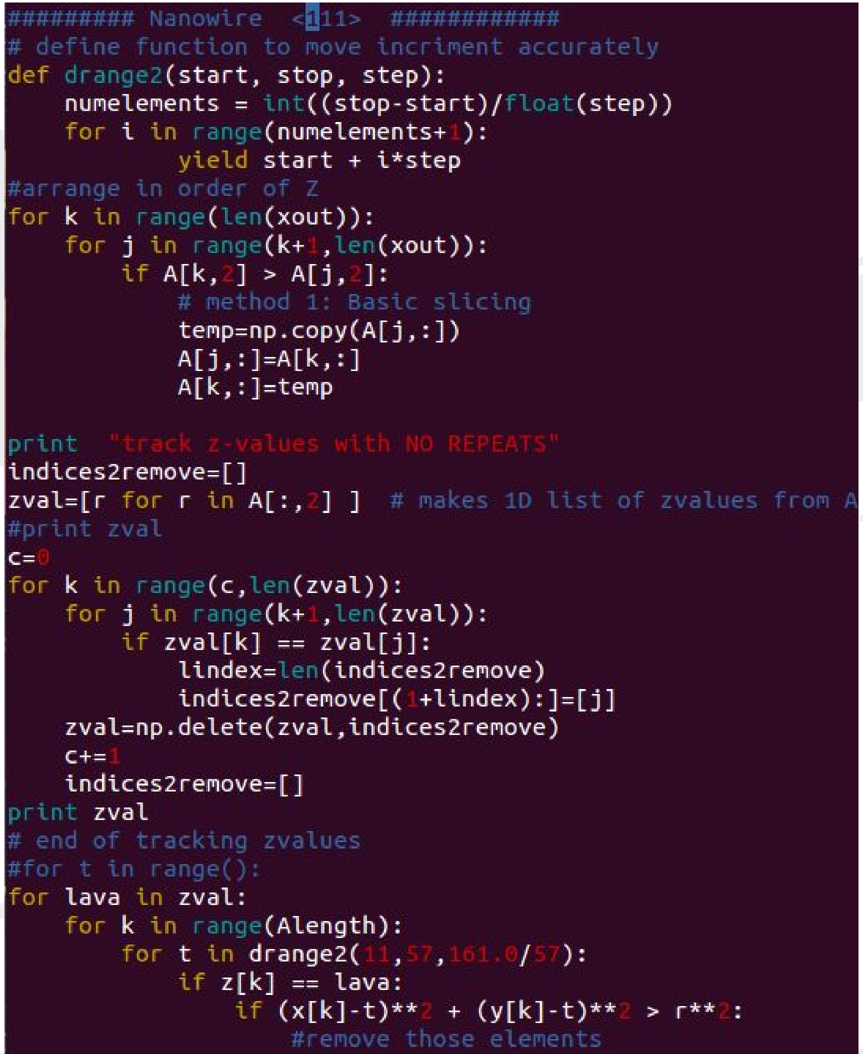
## Creating 001 NW



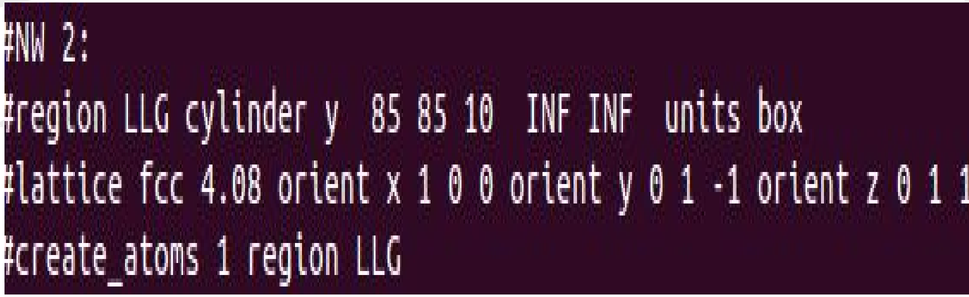
```
A = np.loadtxt('pydump.xyz')
Alength = len(A)
x = A[0:Alength,0]    # first column of data
y = A[0:Alength,1]    # Second column of data
z = A[0:Alength,2]    # third column of data
#Reshape with x=x.reshape(length,1)
x=x.reshape(Alength,1)
y=y.reshape(Alength,1)
z=z.reshape(Alength,1)
#Set Radius of NW r
r = 10   #style metal is in Angostroms
############## Nanowire  <001>  #################
indices2remove=[]
for k in range(Alength):
    if (x[k]-30)**2 + (y[k]-30)**2 > r**2:
        #remove those elements
        #storing indices to an array
        lind2rm=len(indices2remove)
        indices2remove[(1+lind2rm):]=[k]
```



# Creating 011 & 111 NWs



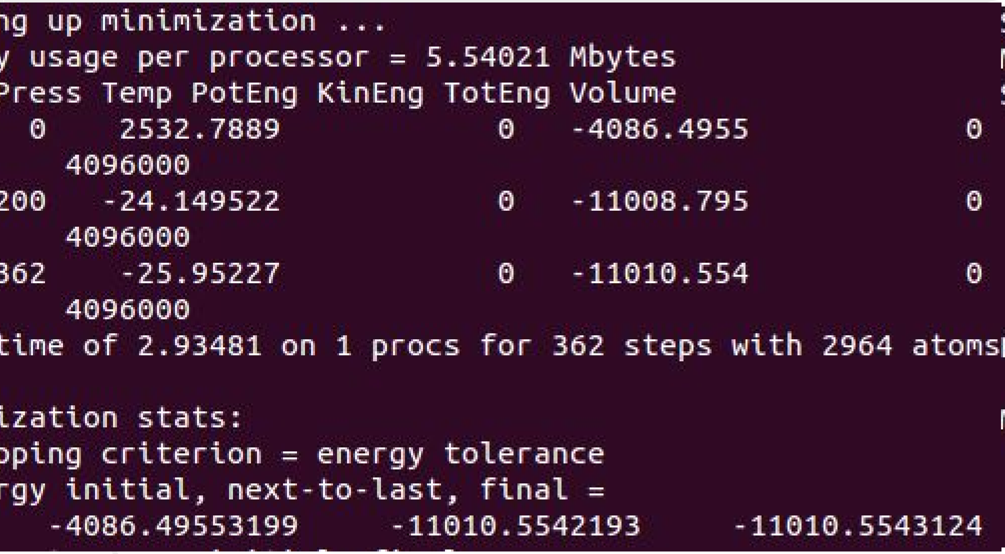
```
######### Nanowire  <111>  ############
# define function to move incriment accurately
def drange2(start, stop, step):
    numelements = int((stop-start)/float(step))
    for i in range(numelements+1):
            yield start + i*step
#arrange in order of Z
for k in range(len(xout)):
    for j in range(k+1,len(xout)):
        if A[k,2] > A[j,2]:
            # method 1: Basic slicing
            temp=np.copy(A[j,:])
            A[j,:]=A[k,:]
            A[k,:]=temp

print  "track z-values with NO REPEATS"
indices2remove=[]
zval=[r for r in A[:,2] ]  # makes 1D list of zvalues from A
#print zval
c=0
for k in range(c,len(zval)):
    for j in range(k+1,len(zval)):
        if zval[k] == zval[j]:
            lindex=len(indices2remove)
            indices2remove[(1+lindex):]=[j]
    zval=np.delete(zval,indices2remove)
    c+=1
    indices2remove=[]
print zval
# end of tracking zvalues
#for t in range():
for lava in zval:
    for k in range(Alength):
        for t in drange2(11,57,161.0/57):
            if z[k] == lava:
                if (x[k]-t)**2 + (y[k]-t)**2 > r**2:
                    #remove those elements
```



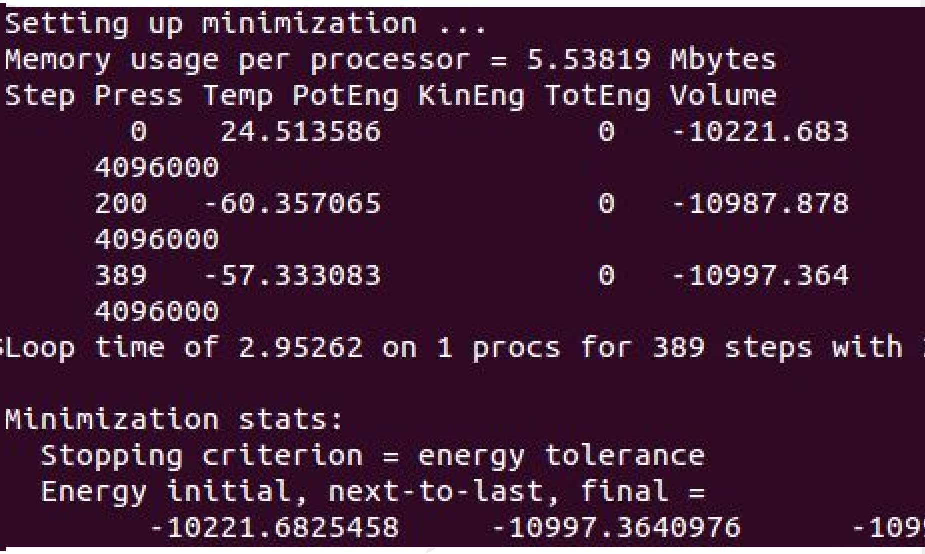
```
#NW 2:
#region LLG cylinder y  85 85 10  INF INF  units box
#lattice fcc 4.08 orient x 1 0 0 orient y 0 1 -1 orient z 0 1 1
#create_atoms 1 region LLG
```

# Energy of 001 & 011

~14eV difference

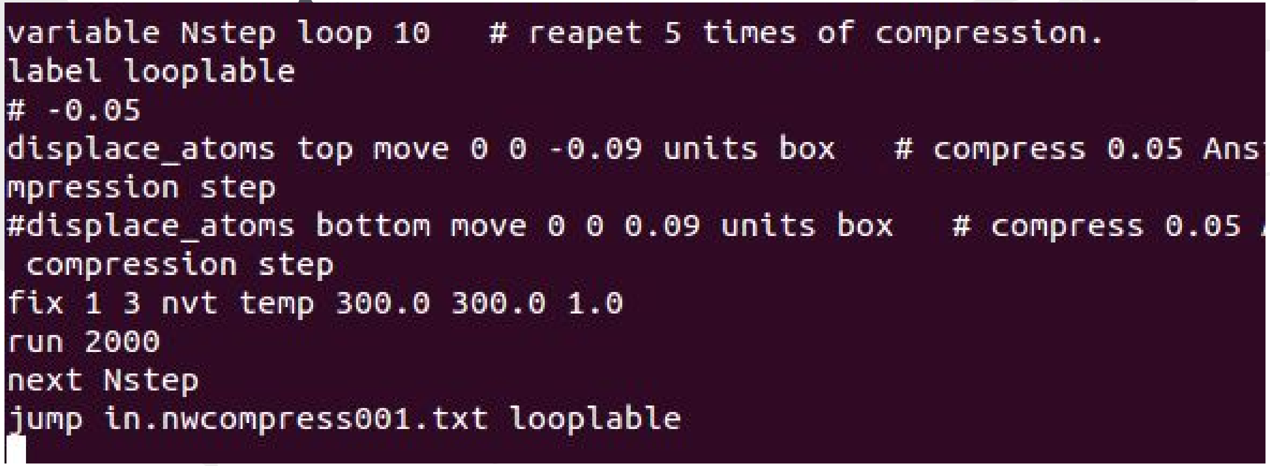


```
ng up minimization ...
y usage per processor = 5.54021 Mbytes
Press Temp PotEng KinEng TotEng Volume
  0    2532.7889             0   -4086.4955           0
    4096000
200   -24.149522             0   -11008.795           0
    4096000
362    -25.95227             0   -11010.554           0
    4096000
time of 2.93481 on 1 procs for 362 steps with 2964 atoms

ization stats:
oping criterion = energy tolerance
rgy initial, next-to-last, final =
   -4086.49553199     -11010.5542193     -11010.5543124
```



```
Setting up minimization ...
Memory usage per processor = 5.53819 Mbytes
Step Press Temp PotEng KinEng TotEng Volume
       0    24.513586             0   -10221.683
     4096000
     200   -60.357065             0   -10987.878
     4096000
     389   -57.333083             0   -10997.364
     4096000
Loop time of 2.95262 on 1 procs for 389 steps with

Minimization stats:
  Stopping criterion = energy tolerance
  Energy initial, next-to-last, final =
        -10221.6825458     -10997.3640976      -109
```

# Compression



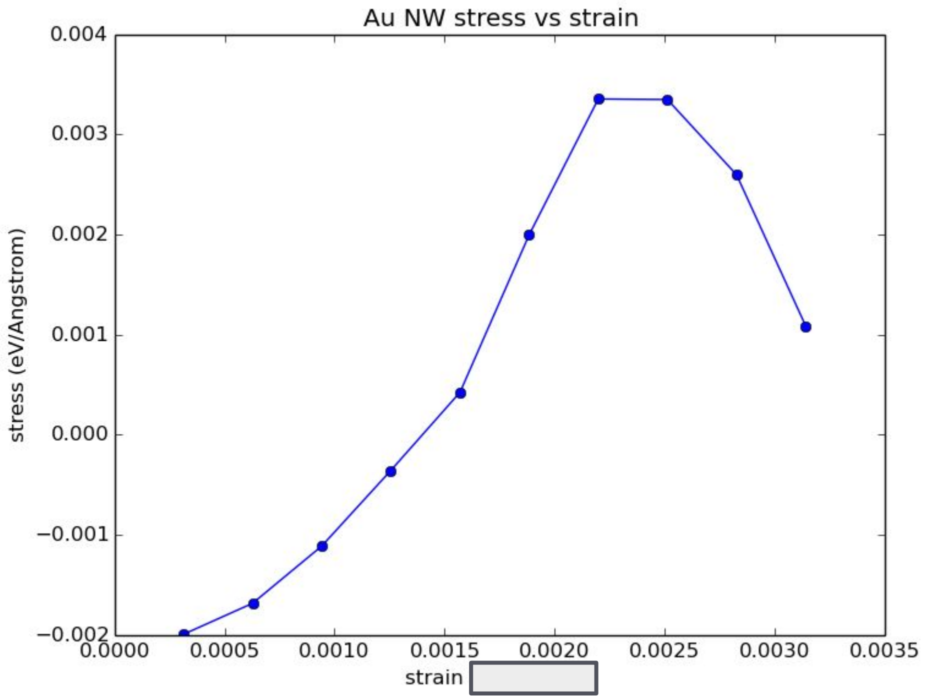
```
variable Nstep loop 10   # reapet 5 times of compression.
label looplable
# -0.05
displace_atoms top move 0 0 -0.09 units box   # compress 0.05 Ans
mpression step
#displace_atoms bottom move 0 0 0.09 units box   # compress 0.05
 compression step
fix 1 3 nvt temp 300.0 300.0 1.0
run 2000
next Nstep
jump in.nwcompress001.txt looplable
```

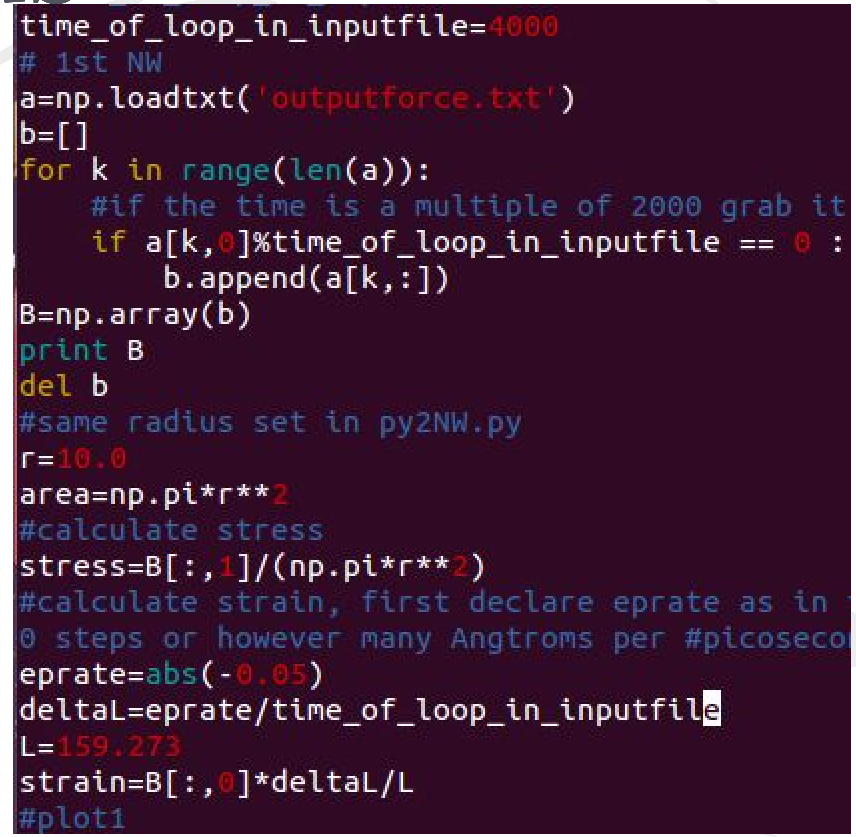
1) https://www.youtube.com/watch?v=jE8En6FZjQU&feature=youtu.be
2) https://www.youtube.com/watch?v=tzJn2lCvGKQ&feature=youtu.be
3) https://www.youtube.com/watch?v=7jjGF-hXtms&feature=youtu.be
4) https://www.youtube.com/watch?v=IiWQjjuVCx4&feature=youtu.be

Video Links

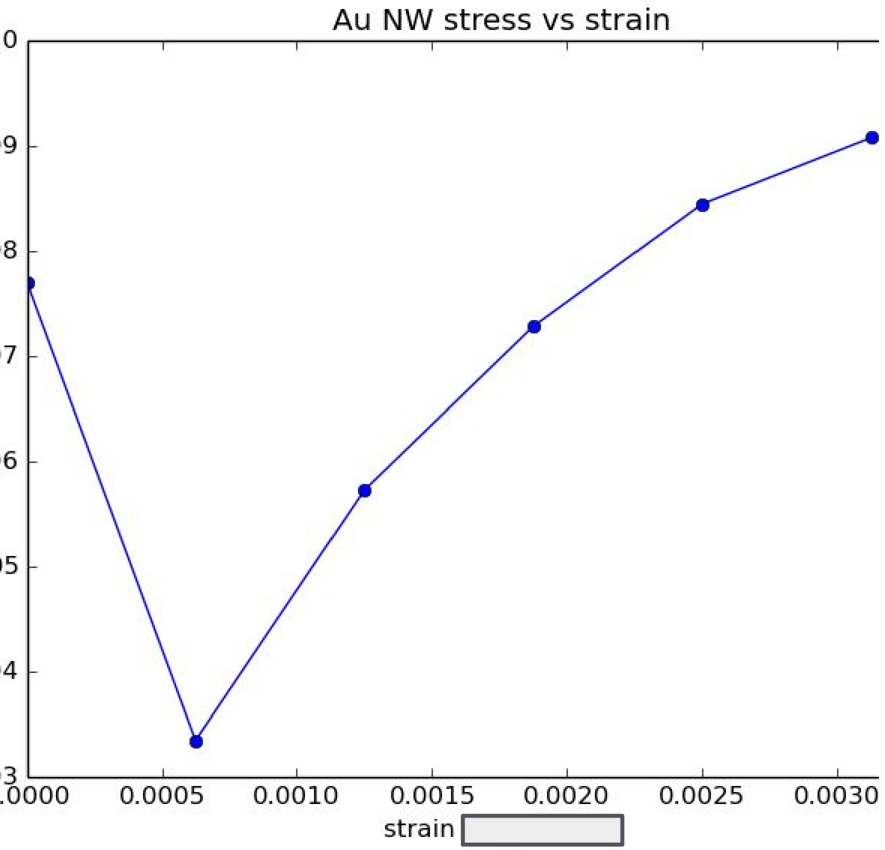
←

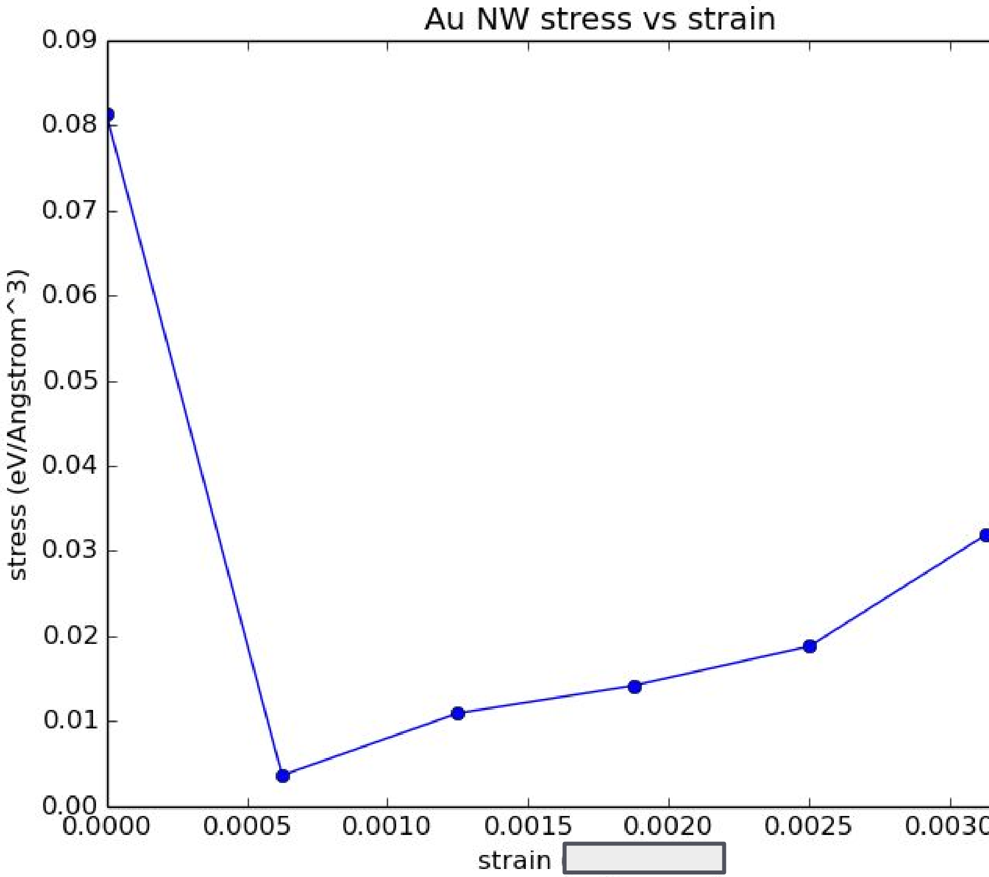
# Young's Modulus




```
time_of_loop_in_inputfile=4000
# 1st NW
a=np.loadtxt('outputforce.txt')
b=[]
for k in range(len(a)):
    #if the time is a multiple of 2000 grab it
    if a[k,0]%time_of_loop_in_inputfile == 0 :
        b.append(a[k,:])
B=np.array(b)
print B
del b
#same radius set in py2NW.py
r=10.0
area=np.pi*r**2
#calculate stress
stress=B[:,1]/(np.pi*r**2)
#calculate strain, first declare eprate as in
0 steps or however many Angtroms per #picoseco
eprate=abs(-0.05)
deltaL=eprate/time_of_loop_in_inputfile
L=159.273
strain=B[:,0]*deltaL/L
#plot1
```

# Moduli r=10,ed=0.1, 001(left) & 011(right)





# Initial Results in eV/Angstrom^3

e4=(stress[4]-stress[1])/(strain[4]-strain[1]) = 2.2388042

e6=(stress[6]-stress[4])/(strain[6]-strain[4]) = 4.6673040

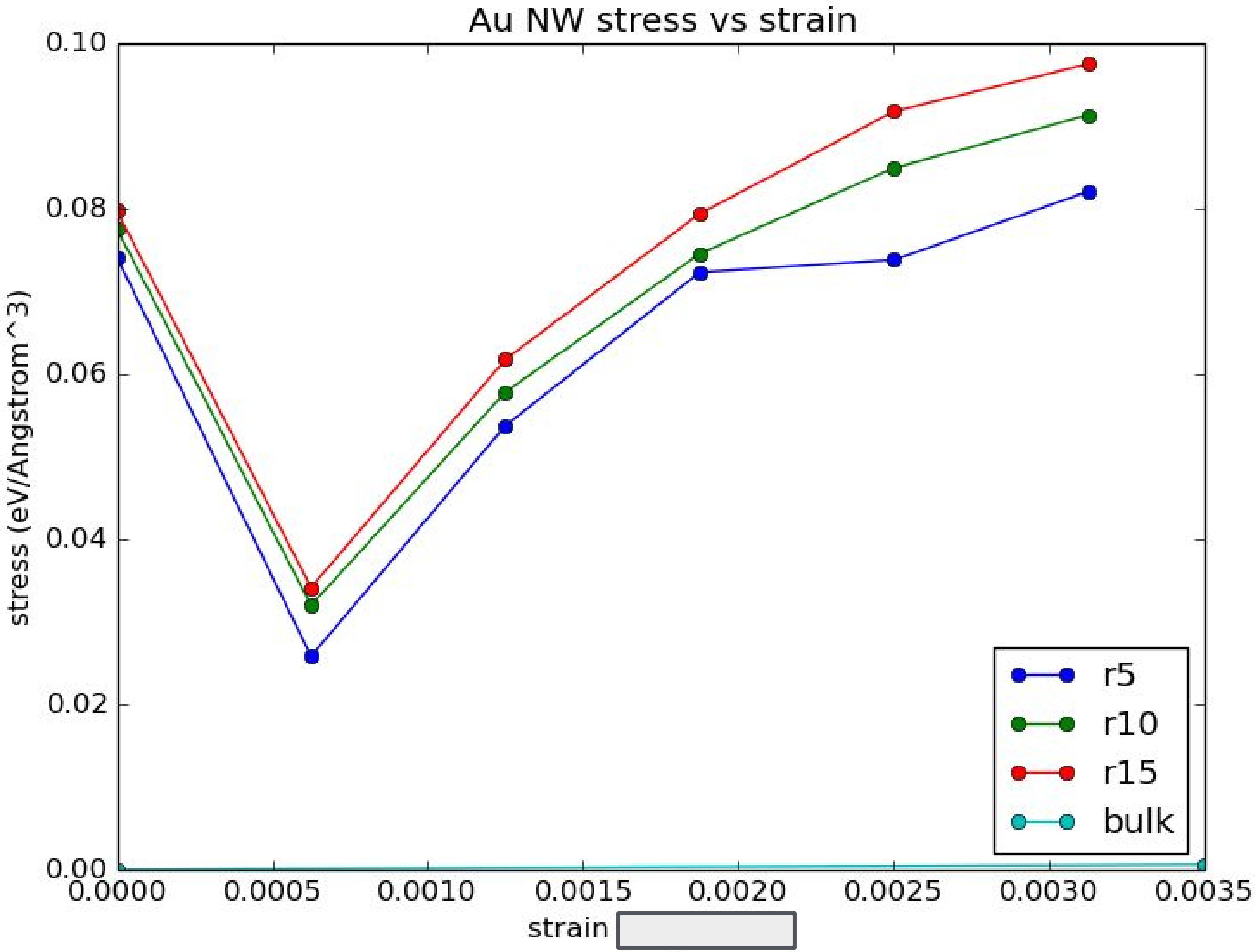
enwavg=3.4530541

ebulk = 0.1715986331

- Bulk Au has E=29GPa or 0.172eV/A^3
- NW Au has E=583.5GPa
- Ratio Enwavg/Ebulk = 20.12850

- Next steps
    - Compare with a different radii NWs
    - Test orientations <011>, <111>

# Comparing Youngs Modulus for different size radii



## Extras

1) https://www.youtube.com/watch?v=0Sw3CaI2u6U&feature=youtu.be
2) https://www.youtube.com/watch?v=dpQ3-waEUT4&feature=youtu.be