NVT(300K)->NVT(100K)

```
variable a loop 5
variable t index 55555 66666 77777 88888 99999
label loop
clear
# Lennard-Jones Melt
#------------Prepare Geometry---------------------------------------------------------
------
units            lj
atom_style       atomic
read_data        LJ_256.in.data
#read_restart    ljNVE.restart.1000000
#------------Initialize Structure-----------------------------------------------------
------
mass             1  1.0
group            Ar type = 1
#------------LJ Potentials-------------------------------------------------------------
------
pair_style       lj/cut 2.5
pair_coeff       * * 1.0 1.0
pair_modify      shift yes
#pair_modify     tail no
#------------Variables-----------------------------------------------------------------
------
#LJ Parameters
variable      kB          equal 1.3806504e-23 # [J/K] Boltzmann
variable      sigma_Ar    equal 3.4e-10        # m
variable      eps_Ar      equal 1.67e-21       # J
variable      mass_Ar     equal 6.63e-26       # kg
variable      tau_Ar      equal 2.1423e-12     # s

variable      T_melt      equal 300*(${kB}/${eps_Ar})
variable      T_0K        equal 0.001
variable      T_run       equal 100*(${kB}/${eps_Ar})
#variable     V           equal vol
variable       dt equal 0.002
#variable     p equal 200 # correlation length
#variable     s equal 10  # sample interval
#variable     d equal $p*$s # dump interval


log log$a.lammps

      #------------ NVT RUN ----------------------------------------------------------
--------------
      velocity            all create ${T_melt} $t dist gaussian mom yes
      fix                 1 all nvt temp ${T_melt} ${T_melt} 10.0
      thermo_style        custom step temp press etotal pe ke vol xlo xhi ylo yhi zlo
zhi
      thermo              500
      timestep            ${dt}
      run                 100000
#     run                 2500
      unfix 1
      #------------ NVT RUN ----------------------------------------------------------
--------------
      fix                 1 all nvt temp ${T_melt} ${T_run} 10.0
      run                 250000
#     run                 2500
      unfix 1
      #------------ NPT RUN ----------------------------------------------------------
--------------
      reset_timestep      0
```

```
        fix              1 all npt temp ${T_run} ${T_run} 10.0 iso 0.0 0.0 10.0
        compute          myDis Ar msd
        dump             xyz all xyz 100000 npt_reheat_dump.$a
        thermo_style     custom step temp press etotal pe ke vol xlo xhi ylo yhi zlo
zhi c_myDis[4]
        thermo           500
        run              250000
#       run              2500
        undump           xyz
        unfix            1
        uncompute        myDis
        #------------ NPT RUN -------------------------------------------------------
--------------
        reset_timestep   0
        fix              1 all npt temp ${T_run} ${T_run} 10.0 iso 0.0 0.0 10.0
        compute          myDis Ar msd
        dump             xyz all xyz 100000 npt_${T_run}_dump.$a
        #----------Calculate Avg Cell Size------------------------------------------
--------------
        variable         myLx equal xhi-xlo
        fix              myLx all ave/time 100 10 1000 v_myLx file Lx.profile$a
        variable         myLx2 equal f_myLx
        thermo_style     custom step temp press etotal pe ke vol xlo xhi ylo yhi zlo
zhi c_myDis[4]
        thermo           500
        run              500000
#       run              10000
        undump           xyz
        unfix            1
        fix              deform all deform 1 x final 0.0 ${myLx2} y final 0.0
${myLx2} z final 0.0 ${myLx2} units box
        run              10000
        unfix            deform
        unfix            myLx
        uncompute        myDis
        #------------ NVT RUN -------------------------------------------------------
--------------
        reset_timestep   0
        fix              1 all nvt temp ${T_run} ${T_run} 10.0
        compute          myDis Ar msd
        thermo_style     custom step temp press etotal pe ke vol xlo xhi ylo yhi zlo
zhi c_myDis[4]
        thermo           500
        run              100000
        uncompute        myDis
        unfix            1
        #------------ kappa ---------------------------------------------------------
--------------
        reset_timestep   0
        fix              1 all nve
        timestep         ${dt}
        compute          myDis Ar msd
        thermo_style     custom step temp press etotal pe ke vol xlo xhi ylo yhi zlo
zhi c_myDis[4]
        thermo           500
        run              250000
#       run              2500
        unfix            1
        uncompute        myDis

        log              log_kappa$a.lammps
        fix              1 all nve
        reset_timestep   0
```

```
        compute              myKE all ke/atom
        compute              myPE all pe/atom
        compute              myStress all stress/atom virial
        compute              flux all heat/flux myKE myPE myStress
        variable             Jx equal c_flux[1]/vol
        variable             Jy equal c_flux[2]/vol
        variable             Jz equal c_flux[3]/vol
        compute              myDis Ar msd
        thermo_style         custom step temp press etotal pe ke vol c_myDis[4] v_Jx
v_Jy v_Jz
        thermo               5
        dump                 xyz all xyz 500000 nve_kappa_dump.$a
        timestep             ${dt}
        run                  2000000
#       run                  2500
        unfix                1
        uncompute            myKE
        uncompute            myPE
        uncompute            myStress
        uncompute            flux

next t
next a
jump in.LJAr.melt loop
```
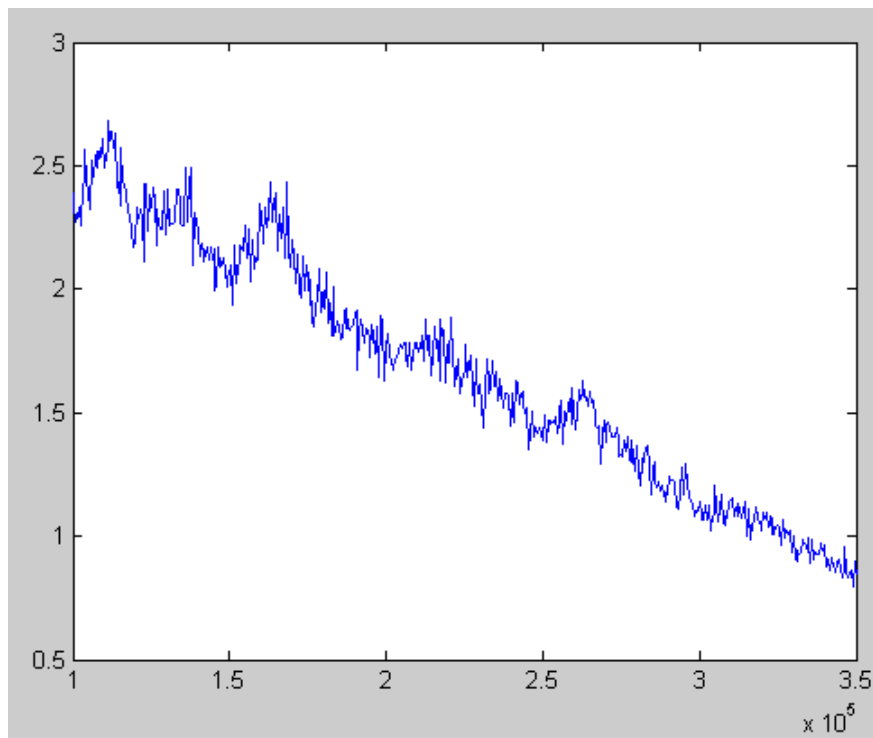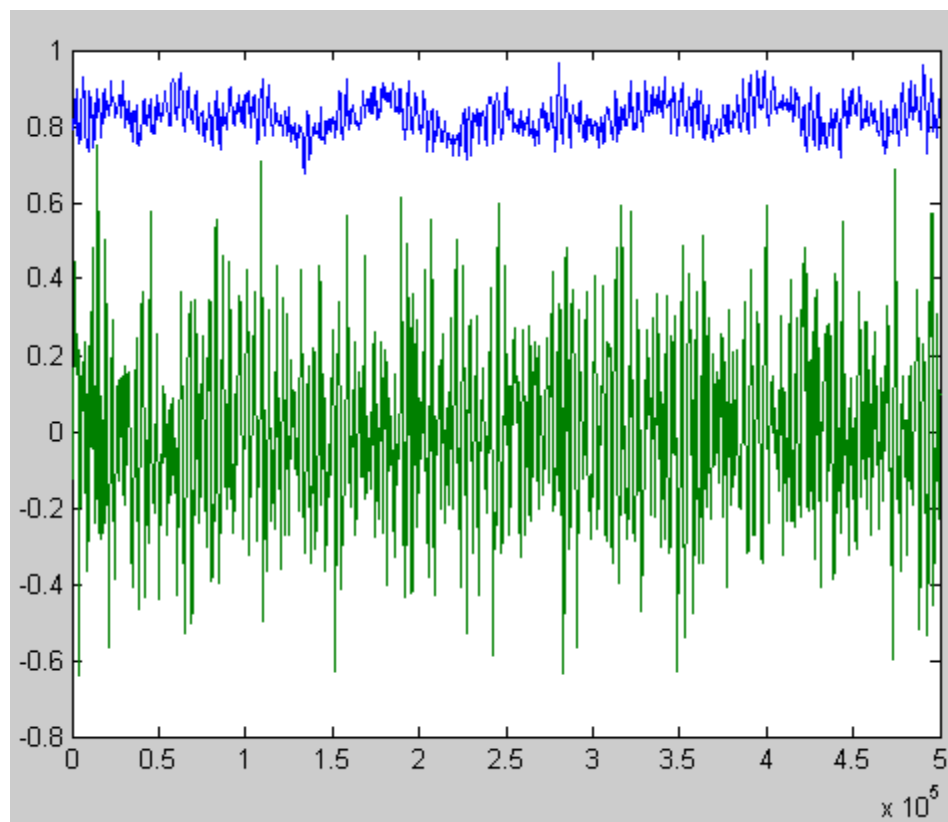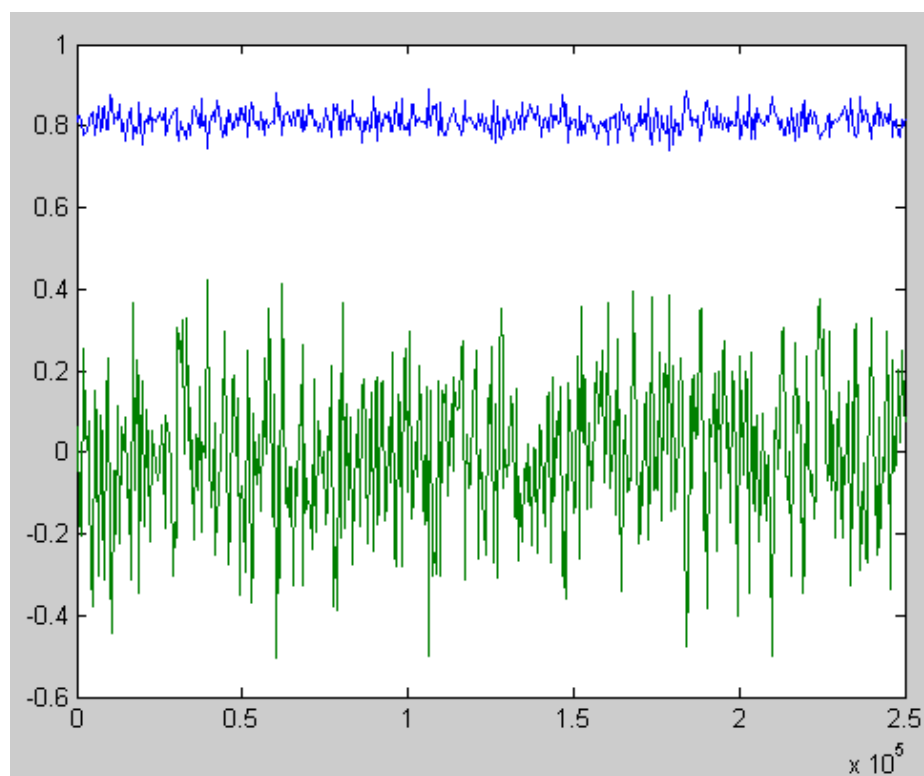

NPT to measure average cell size

NVE

MSD

T = 80K