

```

#----- initialization-----
log          ncl_conta_0.07.log
units        metal
dimension    3
boundary     p f p
atom_style   atomic

variable     w equal 0.07
variable     t equal 100
#-----system definition-----
#Simulation Box

lattice      fcc 5.85
region       box block -0.5 48.5 -1.25 50.5 -0.5
12.5
create_box   2 box

#create atoms

region       A block INF INF -0.75 0.0 INF INF
region       B block 0.5 48.0 0.5 50.0 0.5 12.0
region       C block 17.5 30.5 0.0 12.5 INF INF
region       D block 18 30 0.25 12.5 INF INF
lattice      fcc 25.068
create_atoms 1 region B
delete_atoms region C
lattice      fcc 5.85
create_atoms 1 region D

lattice      fcc 3.615
region       bottom block INF INF -0.75 -0.50 INF
INF
create_atoms 2 region A
lattice      fcc 5.85

mass         1 39.95
mass         2 63.55

group        ar type 1
group        cu type 2
group        bwall region bottom

velocity     all create $t 4928459

#force field

pair_style   lj/cut $(1.0*3.405)

```

```

pair_coeff    1 1 0.0103 3.405 8.5
pair_coeff    2 2 0.41148 2.34 6.5
pair_coeff    1 2 $(v_w*0.06489) 2.872 11.9

neighbor      0.35 bin
neigh_modify  delay 1

timestep      0.005

#Apply fix

shell         mkdir trajectory_w_0.07
shell         cd trajectory_w_0.07

fix           wall bwall setforce 0.0 0.0 0.0
velocity      bwall set 0.0 0.0 0.0
#fix          1 cu spring/self 4.3
#minimize     1.0e-4 1.0e-6 1000 1000

#fix          wall1 all wall/lj126 ylo 0.0 $(v_w*0.06489)
2.872 11.9
#fix          wall1 cu wall/region wall lj126
$(v_w*0.06489) 2.872 11.9
fix           wall2 all wall/reflect yhi EDGE

#fix          3 all nve
#fix          4 all langevin $t $t $(100*dt) 46464678
fix           3 cu nvt temp $t $t $(100*dt)
fix           4 ar nvt temp $t $t $(100*dt)
#fix          4 cu nvt temp $t $t $(10*dt)

compute       arTemp ar temp
compute       cuTemp cu temp
dump          1 all custom 1000 tarj.all_atom.*.txt id
type x y z

thermo        1000
thermo_style   custom step temp c_cuTemp c_arTemp
etotal press
#thermo_modify lost ignore
restart       100000 ncl_data_0.07
run           500000

shell         cd ..
undump        1

```