units metal

echo both

atom\_style atomic

dimension 3

boundary p s p

region box block 0 140 0 100 0 140 units box

create\_box 1 box

lattice fcc 3.61

region cu block 0 140 0 100 0 140 units box

create\_atoms 1 region cu units box

timestep 0.002

pair\_style eam/alloy

pair\_coeff \* \* Cu\_zhou.eam.alloy Cu

# Energy Minimization

minimize 1.0e-4 1.0e-5 10000 10000

# rigid boundary

region 1 block 0 140 0 25 0 140 units box

group anvil1 region 1

region 2 block 0 25 0 100 0 140 units box

group anvil2 region 2

region 3 block 115 140 0 100 0 140 units box

group anvil3 region 3

group anvil union anvil1 anvil2 anvil3

group mobile subtract all anvil

dump 1 all atom 1000 dump.indent8\_3d\_unload.dump.lammpstrj

log log5050\_indent8\_3d\_voidless\_unload.dat

# initial velocities

compute new mobile temp

velocity mobile create 300 482748 temp new

fix 1 mobile nvt temp 300.0 300.0 0.05

fix 2 anvil setforce 0.0 0.0 0.0

# assigning velocity to the indenter in y direction/loading direction

variable y equal "135-step\*dt\*0.1"

print "y is $y"

# indenter position and radius at onset of loading

fix 4 mobile indent 1000.0 sphere 70 v\_y 70 30.0 units box

thermo 100

thermo\_style custom step temp v\_y f\_4[1] f\_4[2] f\_4[3]

run 75000