clear

units metal

dimension 3

processors 3 3 2

boundary p p p

atom\_style atomic

atom\_modify map array

# ---------- Create Atoms ---------------------

lattice fcc 4

Lattice spacing in x,y,z = 4 4 4

region box block 0 20 0 20 0 20 units lattice

create\_box 4 box

Created orthogonal box = (0 0 0) to (80 80 80)

 3 by 3 by 2 MPI processor grid

lattice fcc 4 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1

Lattice spacing in x,y,z = 4 4 4

create\_atoms 4 box

Created 32000 atoms

 create\_atoms CPU = 0.00131922 secs

#replicate 20 20 20

set region box type/fraction 3 0.5 12345

 15736 settings made for type/fraction

set type 4 type/fraction 2 0.5 1

 8188 settings made for type/fraction

set type 3 type/fraction 1 0.5 7214165

 7859 settings made for type/fraction

# ---------- Define Interatomic Potential ---------------------

pair\_style eam/alloy

pair\_coeff \* \* CoFeNiPd.set Co Fe Ni Pd

neighbor 2.0 bin

neigh\_modify every 1 check yes

timestep 0.002 #from jafray 0.002 picometers

velocity all create 2300 12345 mom yes rot yes

# ---------- calculatingcentro symmetry to know whether the atom is distorted or not---------------------

compute csym all centro/atom fcc

compute peratom all pe/atom

compute pattern all cna/atom 3.414

#reset\_timestep 0

thermo 1000

thermo\_style custom step temp etotal ke pe lx ly lz press pxx pyy pzz enthalpy

# ---------- Run Minimization ---------------------

dump 3 all custom 5000 dump.f\* id type x y z vx vy vz fx fy fz c\_csym c\_peratom c\_pattern

fix 3 all npt temp 2300 2300 0.2 iso 0 0 2

run 5000000

Neighbor list info ...

update every 1 steps, delay 10 steps, check yes

 max neighbors/atom: 2000, page size: 100000

 master list distance cutoff = 8.15119

 ghost atom cutoff = 8.15119

 binsize = 4.0756, bins = 20 20 20

 3 neighbor lists, perpetual/occasional/extra = 1 2 0

 (1) pair eam/alloy, perpetual

 attributes: half, newton on

 pair build: half/bin/atomonly/newton

 stencil: half/bin/3d/newton

 bin: standard

 (2) compute centro/atom, occasional

 attributes: full, newton on

 pair build: full/bin/atomonly

 stencil: full/bin/3d

 bin: standard

 (3) compute cna/atom, occasional

 attributes: full, newton on

 pair build: full/bin/atomonly

 stencil: full/bin/3d

 bin: standard

Per MPI rank memory allocation (min/avg/max) = 9.812 | 9.842 | 9.864 Mbytes

Step Temp TotEng KinEng PotEng Lx Ly Lz Press Pxx Pyy Pzz Enthalpy

 0 2300 -113804.31 9513.2494 -123317.56 80 80 80 -241350.62 -241534.27 -241334.72 -241182.86 -190931.59

 1000 2285.1858 -110653.86 9451.975 -120105.83 76.71542 76.71542 76.71542 6043.3015 6927.5626 5850.7661 5351.5756 -108950.87

 2000 2309.9013 -110096.86 9554.2029 -119651.06 76.95438 76.95438 76.95438 -830.50276 -798.79149 -181.66325 -1511.0535 -110333.08

 3000 2312.9673 -109969.63 9566.8848 -119536.52 76.977599 76.977599 76.977599 -526.21434 211.53573 -821.64567 -968.53309 -110119.45

 4000 2297.2754 -110146.53 9501.98 -119648.51 76.948663 76.948663 76.948663 112.79066 -1010.9047 1699.2596 -349.98288 -110114.45

 5000 2307.1446 -110083.67 9542.8006 -119626.47 76.966479 76.966479 76.966479 -896.36651 492.57825 -1799.9305 -1381.7473 -110338.75

 6000 2309.0482 -110112.12 9550.6746 -119662.79 76.953555 76.953555 76.953555 -449.66157 -898.88374 -1191.4751 741.3741 -110240.01

 7000 2299.1335 -109971.23 9509.6653 -119480.89 76.987642 76.987642 76.987642 -530.49761 -1673.5706 270.16436 -188.08662 -110122.32

 8000 2287.9353 -110164.53 9463.3474 -119627.88 76.947826 76.947826 76.947826 -307.80647 -465.39699 -135.75987 -322.26255 -110252.06

 9000 2288.8377 -110168.21 9467.0798 -119635.29 76.926133 76.926133 76.926133 1318.3247 527.84321 2091.6024 1335.5283 -109793.64

 10000 2313.8558 -110015.04 9570.5596 -119585.6 76.980185 76.980185 76.980185 -1345.3421 -794.38413 -1883.121 -1358.5212 -110398.1

 11000 2314.6443 -110081.03 9573.8212 -119654.85 76.957806 76.957806 76.957806 -479.34678 287.41071 -780.27126 -945.17979 -110217.4

 12000 2317.4539 -109954.25 9585.4421 -119539.69 76.978537 76.978537 76.978537 -134.17146 -1264.8346 -60.576761 922.89699 -109992.45

 13000 2300.0277 -110029.73 9513.3641 -119543.09 76.957857 76.957857 76.957857 873.96327 1411.4524 26.003949 1184.4335 -109781.1

 14000 2281.6712 -110105.46 9437.4377 -119542.9 76.995792 76.995792 76.995792 -1555.2303 -744.03872 -2171.0772 -1750.5749 -110548.54

**WARNING: Too many common neighbors in CNA 1 times (../compute\_cna\_atom.cpp:351)**

 15000 2296.129 -110139.4 9497.2382 -119636.64 76.9519 76.9519 76.9519 40.306835 -427.8023 -402.82354 951.54634 -110127.94

 16000 2300.7411 -109979.37 9516.3148 -119495.69 76.985815 76.985815 76.985815 -598.23658 -1197.1643 -1831.3761 1233.8307 -110149.74

 17000 2309.2298 -110071.13 9551.4257 -119622.56 76.951878 76.951878 76.951878 -111.1815 -19.496648 -916.04848 602.00064 -110102.75

 18000 2316.4917 -110118.67 9581.4624 -119700.13 76.934501 76.934501 76.934501 -1.7867523 -362.49686 677.21663 -320.08003 -110119.18

 19000 2309.8031 -110054.41 9553.797 -119608.2 76.958645 76.958645 76.958645 -266.58199 -1128.8355 -364.56744 693.65701 -110130.25

 20000 2293.6371 -110102.8 9486.9311 -119589.73 76.987752 76.987752 76.987752 -1529.108 -1136.4134 -1911.3066 -1539.6042 -110538.31

 21000 2285.317 -110097.22 9452.5178 -119549.73 76.985898 76.985898 76.985898 -1188.6027 -2155.7194 -85.947785 -1324.1408 -110435.72

 22000 2283.8414 -110214.95 9446.4142 -119661.36 76.937457 76.937457 76.937457 -13.736644 -273.12968 -464.343 696.26275 -110218.85

 97,1 0