

The input file for the LAMMPS code to simulate the nanoindentation on the (110)Si at a temperature of 300 K is listed as follows:

```

units                metal
boundary             p m p
atom_style           atomic
neighbor             4 bin
neigh_modify         delay 5
lattice              diamond 5.431
read_data            data.txt
pair_style            atomistica BrennerScr
pair_coeff            * * Si Si Si
group subin          type 1
group fixatom        type 2
group thermatom      type 3
group                sub union subin fixatom thermatom
fix                  subin nve
fix                  6 fixatom setforce 0 0 0
fix                  7 fixatom nve
velocity             fixatom set 0 0 0 units box
fix                  9 thermatom langevin 300 300 0.1 89994827 tally yes
fix                  10 thermatom nve
variable             yy equal "408.70-step*0.002"
fix                  8 all indent 10.0 sphere 325.86 v_yy 326.041 100 units box
thermo               50
timestep             0.0025
thermo_style         custom elapsed temp f_8[1] f_8[2] f_8[3]
dump                 1 all cfg 500 dump.indentation.*.cfg mass type xs ys zs type vx vy vz
dump_modify          1 element Si Si Si
dump_modify          1 first yes
dump_modify          1 sort id
run                  30000

```