

```

#initialization
units      metal
dimension  2
boundary    p p p
atom_style  full
variable    t equal 3000
variable    a equal 1.42
variable    d equal 0.015
variable    xdim equal 183
variable    ydim equal 18
variable    delT equal 40

lattice      custom 1.0 &
             a1 $(1.5*v_a) $(0.5*sqrt(3)*v_a) 0.0 &
             a2 $(1.5*v_a) $(-0.5*sqrt(3)*v_a) 0.0 &
             basis 0.0 0.0 0.0 &
             basis $(1/3) $(1/3) 0.0

region       mybox block 0 $(v_xdim) 0 $(v_ydim) -
0.25 0.25
create_box   1 mybox
create_atoms 1 box
pair_style    tersoff/table
pair_coeff    * * SiCGe.tersoff C
mass          1 12
velocity      all create $t 4587125

group         carbon type 1
variable      left equal $(bound(carbon,xmin)/4.26)+0.51
variable      right equal $(bound(carbon,xmax)/4.26)-0.51
region        l_edge block INF $(v_left) INF INF INF
INF
region        r_edge block $(v_right) INF INF INF
INF INF
group         ledge region l_edge
group         redge region r_edge
region        defect block $(v_xdim/2) $(v_right-
3.0) INF INF INF INF
delete_atoms   porosity defect $(v_d) 4857549

timestep      0.00025

fix           fl ledge setforce 0.0 0.0 0.0
fix           fr redge setforce 0.0 0.0 0.0
velocity      ledge set 0.0 0.0 0
velocity      redge set 0.0 0.0 0

```

```

fix           1 all npt temp $t $t $(100*dt) iso 0.0 0.0
$(100*dt)
write_data    data_at_*.out
thermo        1000
run           3000000

unfix         1

#shell        mkdir trajectory_tr
#shell        cd trajectory_tr
#fix          1 all nvt temp $t $t $(100*dt)
#thermo       100
#dump         1 all custom 100 tarj.all_atom.*.txt id type
x y z
#run          2000000000

#unfix        1

fix           1 all nve

region        lbath block $(v_left) $(v_left+3.0)
INF INF INF INF
region        rbath block $(v_right-3.0) $(v_right)
INF INF INF INF
region        middle block $(v_left+4) $(v_right-4)
INF INF INF INF
group         latom region lbath
group         ratom region rbath
group         matom region middle
fix           lheat latom nvt temp $(v_t+v_delT/2)
$(v_t+v_delT/2) $(100*dt)
fix           rheat ratom nvt temp $(v_t-v_delT/2) $(v_t-
v_delT/2) $(100*dt)

compute       ltemp latom temp
compute       rtemp ratom temp
compute       mtemp matom temp

thermo_style   custom step temp c_ltemp c_mtemp
c_rtemp press vol
thermo        1000
run           2000000000

```