

Graphene

```
##### Initialization #####
variable project string graphene
variable t equal 300.0 # temperature (K)

log          ${project}_log.txt
units        metal # grams/mole, angstroms, ps, eV, K, bars, gm/cm^3
dimension    2
boundary     p p p
atom_style   atomic

# Building the graphene structure

variable l equal 1.42 # bond length in angstroms
variable m equal 20 # number of unit cells along length
variable n equal 20 # number of unit cells along width
variable L equal $(sqrt(3)*v_l*v_m) # length of the graphene sheet
variable W equal $(3*v_l*v_n) # width of the graphene sheet

region box block 0 ${L} 0 ${W} -10 10 units box
create_box 1 box
mass 1 12.01 # mass of carbon atom

lattice custom ${l} &
  a1 $(sqrt(3)) 0.0 0.0 &
  a2 0.0 3.0 0.0 &
  basis 0.0 0.0 0.0 &
  basis $(1/2) $(1/6) 0.0 &
  basis $(1/2) $(1/2) 0.0 &
  basis 0.0 $(2/3) 0.0
region mybox block 0 ${L} 0 ${W} -0.1 0.1 units box
create_atoms 1 region mybox

velocity all create $t 12345 dist gaussian

# Definition of interatomic potential
pair_style tersoff/table
pair_coeff * * SiCGe.tersoff C

# Simulation settings
timestep 0.00025
neighbor 3.0 bin
neigh_modify delay 0 every 1 check yes
```

```
min_style cg
minimize 1e-10 1e-12 10000 100000

write_data ${project}_data.txt

# Equilibration
fix 1 all nvt temp $t $t $(100.0*dt)
thermo 100
thermo_style custom step temp etotal press
dump 1 all custom 100 ${project}_dump.txt id type x y z vx vy vz
run 200000
```

Silicone

```
##### Initialization #####
variable project string silicon
variable t equal 300.0 # temperature (K)

log          ${project}_log.txt
units        metal # grams/mole, angstroms, ps, eV, K, bars, gm/cm^3
dimension    3
boundary     p p p
atom_style   atomic

# loading the silicone structure

read_data si_supercell.data

velocity all create $t 12345 dist gaussian

# Definition of interatomic potential
pair_style sw
pair_coeff * * Si.sw Si

# Simulation settings
timestep 0.00025
neighbor 3.0 bin
neigh_modify delay 0 every 1 check yes

min_style cg
minimize 1e-10 1e-12 10000 100000

write_data ${project}_data.txt

# Equilibration
fix 1 all nvt temp $t $t $(100.0*dt)
thermo 100
thermo_style custom step temp etotal press
dump 1 all custom 100 ${project}_dump.txt id type x y z vx vy vz
run 20000
```

hBN-Stanene

```
##### Initialization #####
variable project string hbn_sn
variable t equal 300.0 # temperature (K)

log          ${project}_log.txt
units        metal # grams/mole, angstroms, ps, eV, K, bars, gm/cm^3
dimension    3
boundary     p p p
atom_style   atomic

# Building the hbn-sn structure

variable L equal 40.0 # length of the hbn-sn sheet
variable W equal 40.0 # width of the hbn-sn sheet

region box block 0 ${L} 0 ${W} -10 10 units box
create_box 3 box
mass 1 10.811 # mass of boron atom
mass 2 14.007 # mass of nitrogen atom
mass 3 118.71 # mass of tin atom

# building hbn
variable lbn equal 1.45 # bond length in angstroms
lattice custom 1 &
  a1 $(sqrt(3)*v_lbn) 0.0 0.0 &
  a2 0.0 $(3.0*v_lbn) 0.0 &
  a3 0.0 0.0 1.0 &
  basis 0.0 0.0 0.0 &
  basis $(1/2) $(1/6) 0.0 &
  basis $(1/2) $(1/2) 0.0 &
  basis 0.0 $(2/3) 0.0
region bnbx block 0 ${L} 0 ${W} -0.5 0.0 units box
create_atoms 1 region bnbx basis 2 2 basis 4 2

# building sn
variable lsn equal 2.69 # planar bond length in angstroms
variable hsn equal 0.88 # buckling height of sn atom in angstroms
lattice custom 1 &
  a1 $(sqrt(3)*v_lsn) 0.0 0.0 &
  a2 0.0 $(3.0*v_lsn) 0.0 &
  a3 0.0 0.0 $(-2*v_hsn) &
  basis 0.0 0.0 0.0 &
  basis $(1/2) $(1/6) $(1/2) &
```

```

basis $(1/2) $(1/2) 0.0 &
basis 0.0 $(2/3) $(1/2)
region snbox block 0 ${L} 0 ${W} 3.0 5.0 units box
create_atoms 3 region snbox
velocity all create $t 12345 dist gaussian

# Definition of interatomic potential
pair_style hybrid tersoff tersoff lj/cut 10.0
pair_coeff * * tersoff 1 BNC.tersoff B N NULL
pair_coeff * * tersoff 2 Sn.tersoff NULL NULL Sn
pair_coeff 1 3 lj/cut 0.0138 4.23 10
pair_coeff 2 3 lj/cut 0.00857 4.026 10

# Simulation settings
timestep 0.00025
neighbor 3.0 bin
neigh_modify delay 0 every 1 check yes

min_style cg
minimize 1e-10 1e-12 10000 100000

write_data ${project}_data.txt

# Equilibration
fix 1 all nvt temp $t $t $(100.0*dt)
thermo 100
thermo_style custom step temp etotal press
dump 1 all custom 100 ${project}_dump.txt id type x y z vx vy vz
run 20000

```

Carbon NanoTube

```
# Initial setup for Carbon Nanotube (CNT) simulation in LAMMPS
variable project string cnt
variable t equal 298 # temperature (K)

log          ${project}_log.txt
units        metal # grams/mole, angstroms, ps, eV, K, bars, gm/cm^3
dimension    3
boundary      p p p
atom_style    atomic

# Building the graphene structure

variable l equal 1.42 # bond length in angstroms
variable m equal 15 # number of unit cells in along circumferential direction
variable n equal 20 # number of unit cells along axial direction
variable L equal $(sqrt(3)*v_l*v_m) # length of the graphene sheet
variable W equal $(3*v_l*v_n) # width of the graphene sheet

region box block 0 ${L} -10 10 0 ${W} units box
create_box 1 box
mass 1 12.01 # mass of carbon atom

# Generating graphene sheet
lattice custom ${l} &
  a1 $(sqrt(3)) 0.0 0.0 &
  a2 0.0 1.0 0.0 &
  a3 0.0 0.0 3.0 &
  basis 0.0 0.0 0.0 &
  basis $(1/2) 0.0 $(1/6) &
  basis $(1/2) 0.0 $(1/2) &
  basis 0.0 0.0 $(2/3)
region graphenebox block 0 ${L} -0.1 0.1 0 ${W} units box
create_atoms 1 region graphenebox

# creating cnt from graphene

variable R equal ${L}/(2*3.14159265359) # radius of the CNT
variable cx equal (xlo+xhi)/2.0 # center of the CNT
variable cy equal (ylo+yhi)/2.0 # center of the CNT

# setting up loop for displacing atoms
variable natoms equal count(all)
variable id loop ${natoms}
```

```

label loop

group anatom id ${id}
variable x equal xcm(anatom,x)
variable y equal xcm(anatom,y)

variable theta equal  $$(v\_x^2 * 3.1416 / lx)$ 

variable newx equal  $$(v\_R * \cos(v\_theta) + v\_cx)$ 
variable newy equal  $$(v\_R * \sin(v\_theta) + v\_cy)$ 

variable dx equal  $$(v\_newx - v\_x)$ 
variable dy equal  $$(v\_newy - v\_y)$ 

displace_atoms anatom move v_dx v_dy 0.0 units box
group anatom delete
next id
jump SELF loop

velocity all create $t 12345 dist gaussian

# Definition of interatomic potential
pair_style tersoff/table
pair_coeff * * SiCGe.tersoff C

# Simulation settings
timestep 0.00025
neighbor 3.0 bin
neigh_modify delay 0 every 1 check yes

min_style cg
minimize 1e-10 1e-12 10000 100000

write_data ${project}_data.txt

# Equilibration
fix 1 all nvt temp $t $t  $$(100.0 * dt)$ 
thermo 100
thermo_style custom step temp etotal press
dump 1 all custom 100 ${project}_dump.txt id type x y z vx vy vz
run 2000

```

Droplet

```
# Initial setup
variable project string droplet
variable t equal 90 # temperature (K)

log          ${project}_log.txt
units        metal # grams/mole, angstroms, ps, eV, K, bars, gm/cm^3
dimension    3
boundary     p p f
atom_style   atomic

# Building the graphene structure

variable l equal 50.0 # length of a the cubic droplet side
variable L equal $(4*v_l) # length of the simulation box in x direction
variable W equal $(v_l) # length of the simulation box in y direction
variable H equal $(5*v_l) # length of the simulation box in z direction

region box block 0 ${L} 0 ${W} 0 ${H} units box
create_box 2 box
mass 1 39.948 # mass of argon atom
mass 2 63.546 # mass of copper atom

# Generating copper plate
lattice fcc 3.610
region plate block 0 ${L} 0 ${W} 0 5 units box
create_atoms 2 region plate

# Generating argon vapor
lattice fcc 25.068
region vapor block 0 ${L} 0 ${W} 5 ${H} units box
create_atoms 1 region vapor

# Generating cubic droplet
region droplet block $(v_L/2.0-v_l/2.0) $(v_L/2.0+v_l/2.0) &
$(v_W/2.0-v_l/2.0) $(v_W/2.0+v_l/2.0) &
5 $(5+v_l) units box
delete_atoms region droplet
lattice fcc 5.85
create_atoms 1 region droplet

velocity all create $t 12345 dist gaussian

# Definition of interatomic potential
```

```

pair_style hybrid eam lj/cut 10.0
pair_coeff 2 2 eam Cu_u3.eam
pair_coeff 1 1 lj/cut 0.0103 3.405 8.5
pair_coeff 1 2 lj/cut $(0.03*0.06489) 2.872 11.9

# Simulation settings
timestep 0.00025
neighbor 3.0 bin
neigh_modify delay 0 every 1 check yes
# applying reflective boundary conditions at the top of the box
fix wall1 all wall/reflect zhi EDGE
# fixing the bottom layer of the copper plate
region bottom block 0 ${L} 0 ${W} 0 1 units box
group bottom region bottom
fix bwall bottom setforce 0.0 0.0 0.0
velocity bottom set 0.0 0.0 0.0
group mobile subtract all bottom

write_data ${project}_data_init.txt

min_style cg
minimize 1e-10 1e-12 10000 100000

write_data ${project}_data.txt

# Equilibration
compute Tmobile mobile temp
fix 1 mobile nvt temp $t $t $(100.0*dt)
thermo 1000
thermo_style custom step temp etotal press
thermo_modify temp Tmobile
dump 1 all custom 1000 ${project}_dump.txt id type x y z vx vy vz
run 200000

```