Computersimulation in der Materialwissenschaft

WS 2014-2015

Diplom Werkstoffwissenschaft + andere Interessenten

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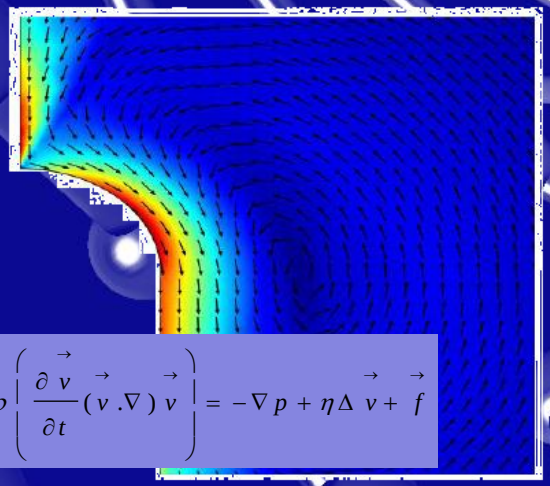
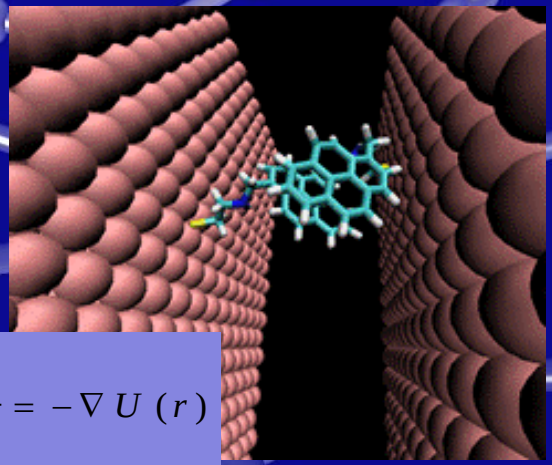
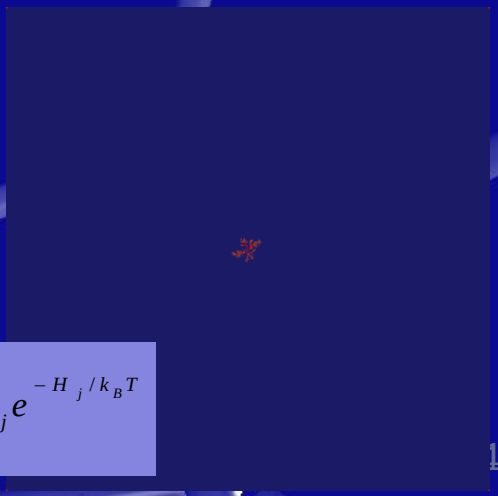
ORT: SCH/A316/H



$$\rho\left(\frac{\partial \vec{v}}{\partial t}(\vec{v}.\nabla)\vec{v}\right) = -\nabla p + \eta\Delta\vec{v} + \vec{f}$$



$$m\frac{d^2 r}{dt^2} = -\nabla U(r)$$



$$\frac{1}{Z}\sum_j A_j e^{-H_j/k_B T}$$

Topic:

Molecular Dynamics Simulations

Outline:

Part I. Molecular Dynamics and LAMMPS code

Part II. Application 1: Melting and cooling of nanostructures

Part III. Application 2: Mechanical stress and Electron beam irradiation

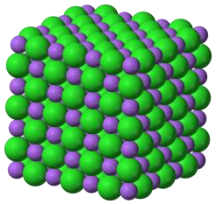
Part I:

Molecular Dynamics and LAMMPS code

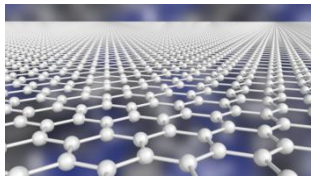
Basic concepts

Molecular Dynamics (MD) is a computational method to predict the movement of an atom under a force contributed by other atoms.

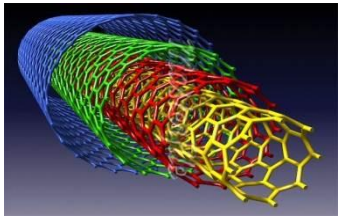
What we can study with MD?



0D materials

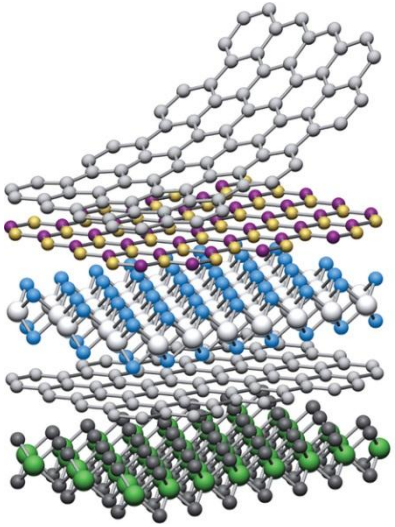


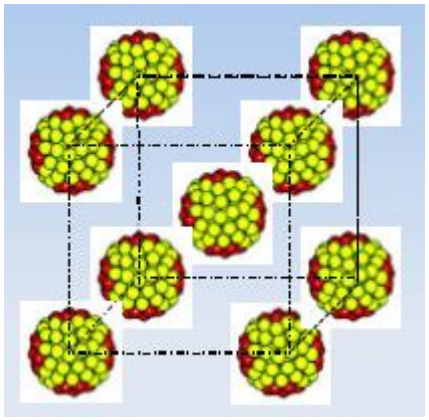
2D materials



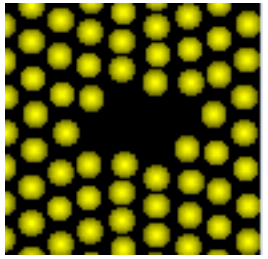
Nanotubes and nanowires

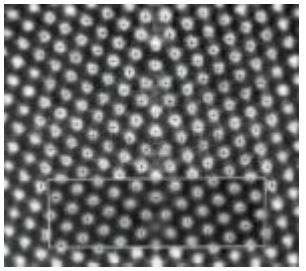
Low-dimensional systems





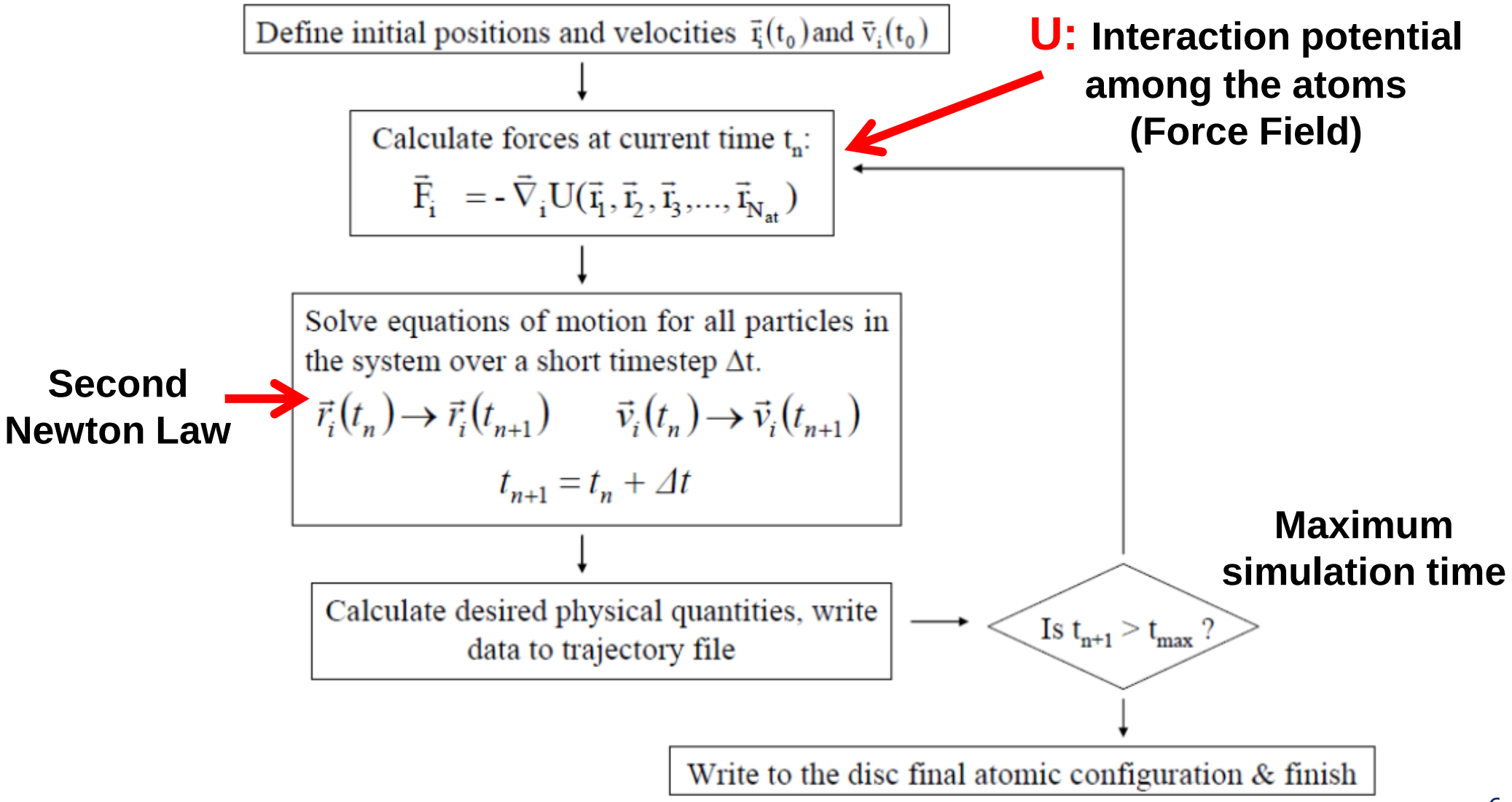
Heterostructures





Defects

Algorithm for MD



Molecular Dynamics

How could we perform a MD simulation?

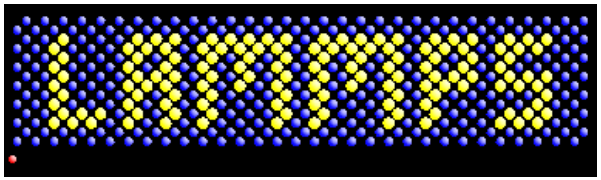
Private code

We can develop our own MD code employing:

- C++
- Python
- Fortran
- Java, etc.

Open source code

Free access.



NAMD
Scalable Molecular Dynamics

GROMACS FAST. FLEXIBLE. FREE.

Commercial code

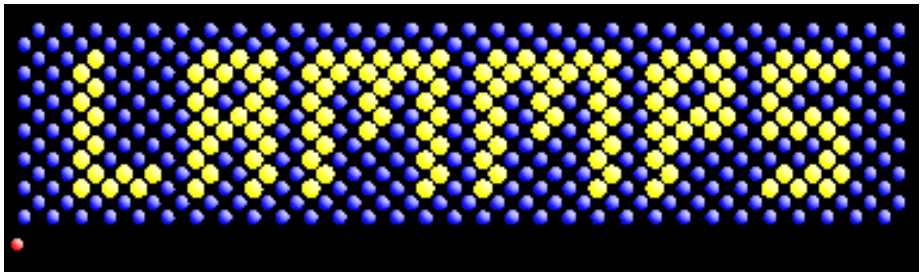
You have to pay for it.

Amber

accelrys®

MATERIALS STUDIO

Molecular Dynamics Simulations
HARMM

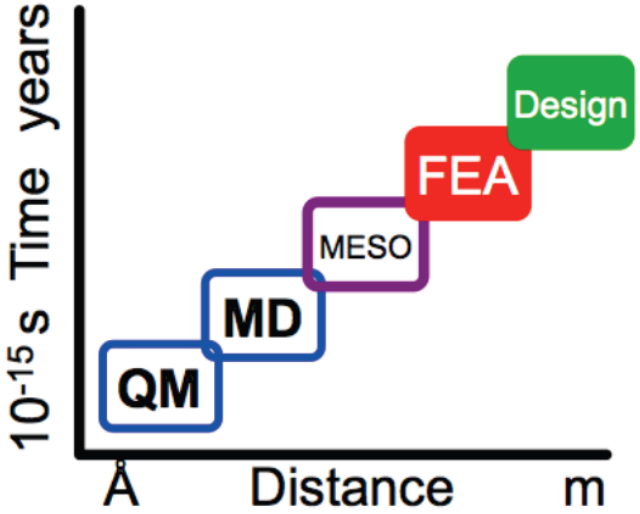


LAMMPS: Large-scale Atomic/Molecular Massively Parallel Simulator

LAMMPS code

Scope:

- Classical molecular dynamics (MD) code.
- Open source, highly portable C++.
- Run in serial or parallel.
- Easy to download, install and run !!!

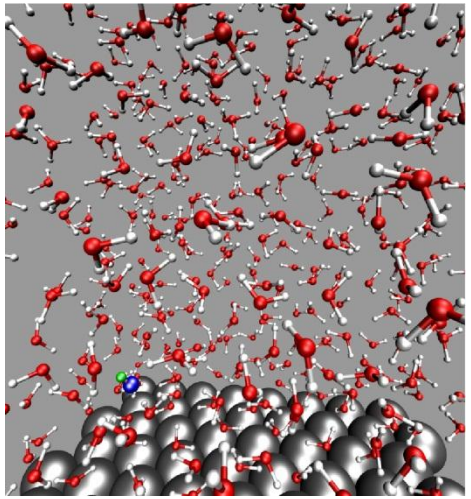


- Atomistic, mesoscale and coarse-grain simulations.
- Three primary communities are supported by force fields, boundary conditions and diagnostics:
  - Biomolecules and polymers (soft materials)
  - Solids materials science
  - Mesoscale to continuum

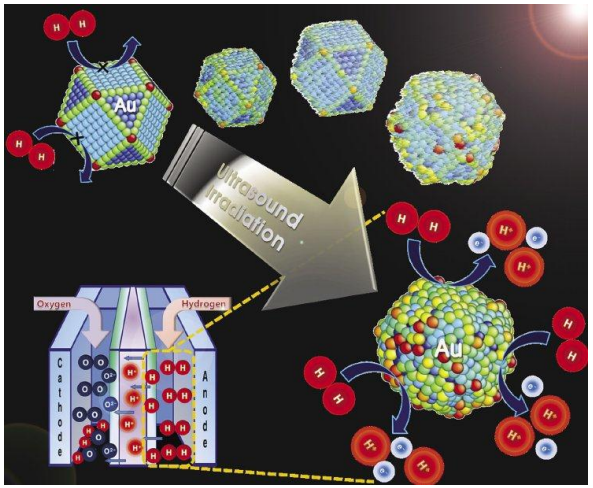
LAMMPS code

Overview

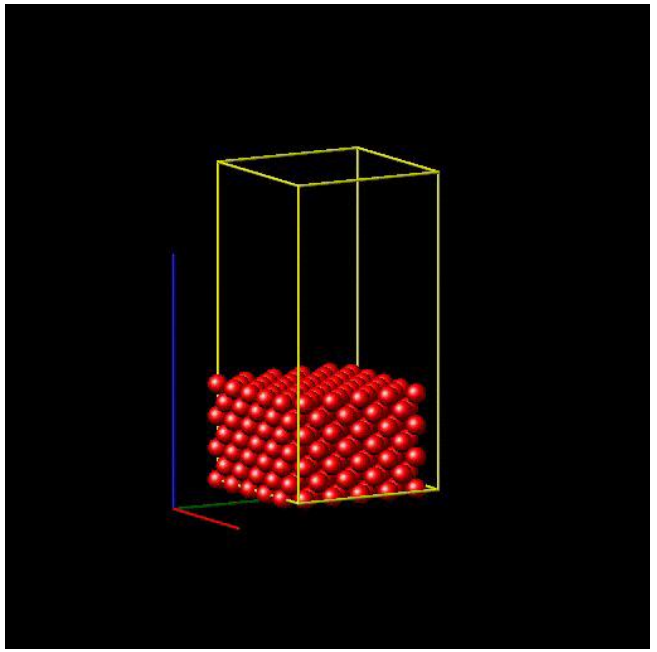
Electrochemical absorption of OH



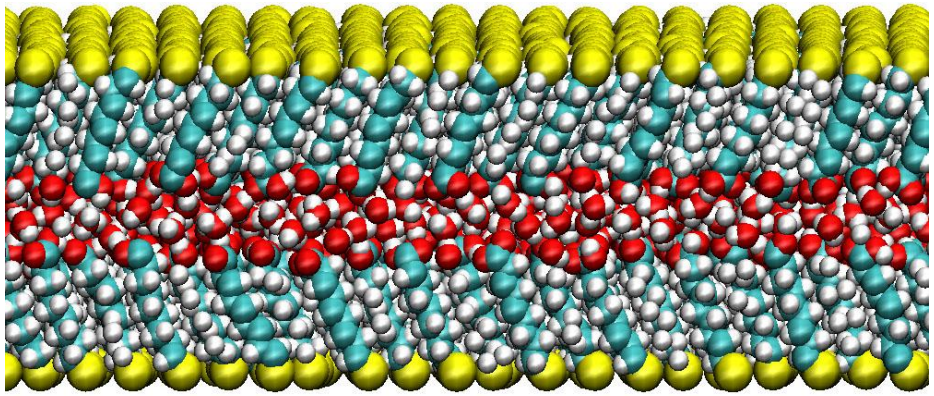
Electrocatalytic activity of gold nanoparticles



Chemical vapor deposition



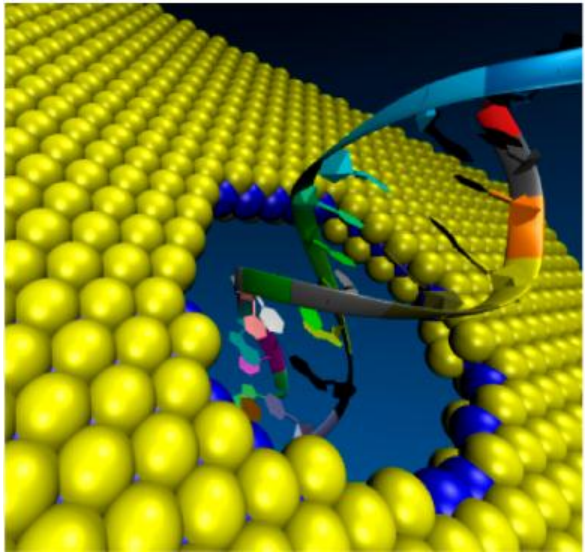
Self-assembled monolayers



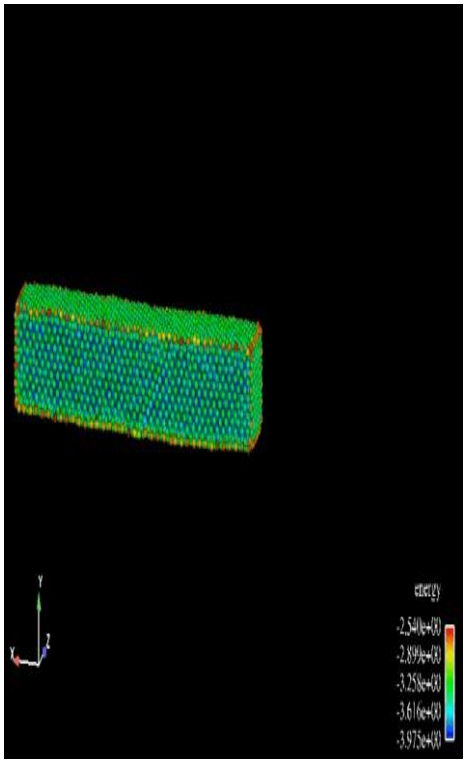
LAMMPS code

Overview

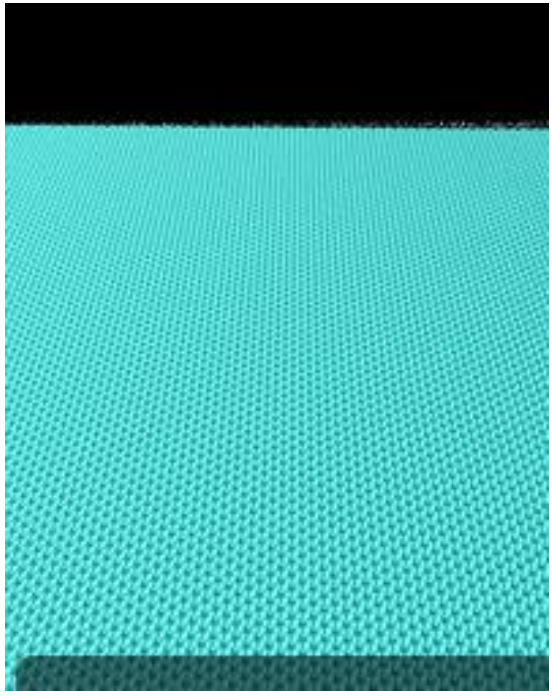
DNA base detection



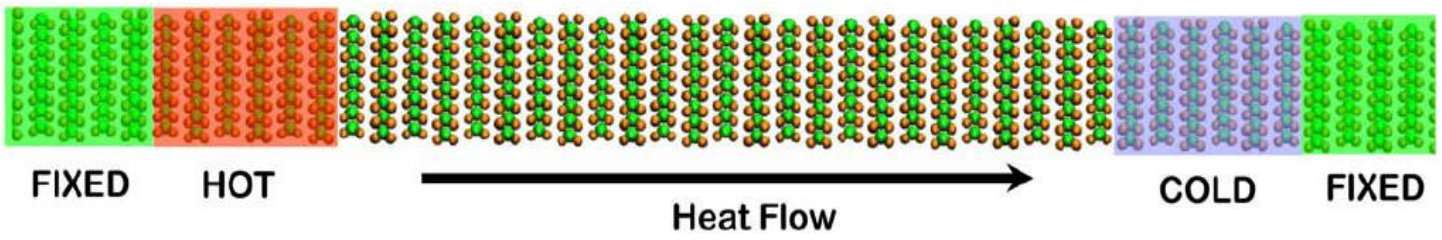
Growth of nanowires



Electron beam irradiation

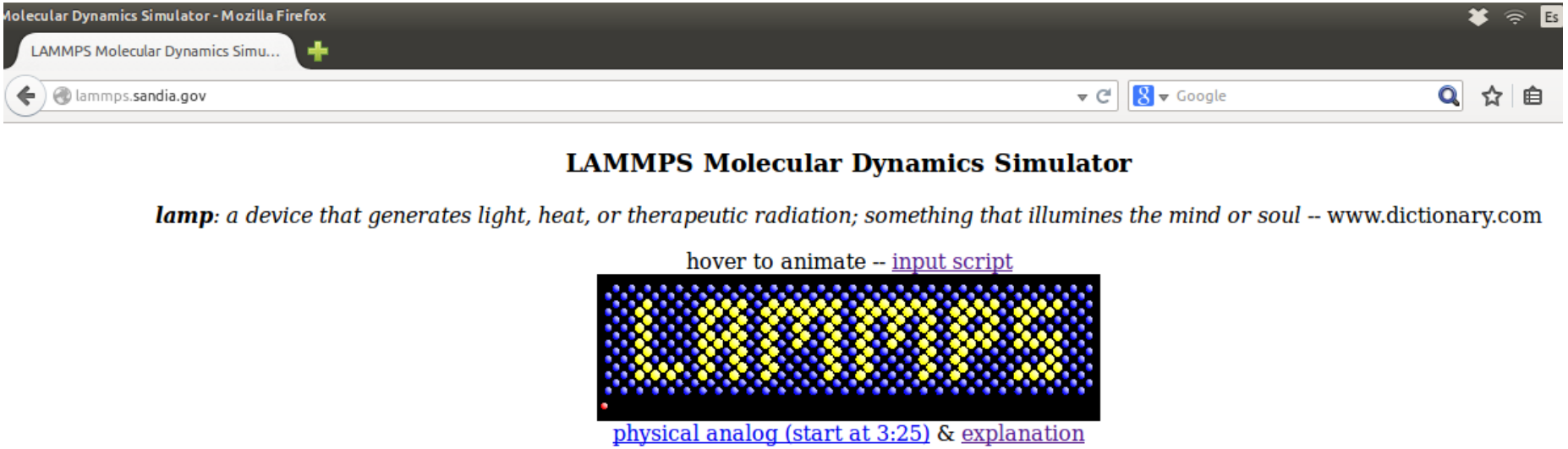


Thermal transport in nanomaterials



How could I get this code?

URL: lammps.sandia.gov



INPUT file

Commands

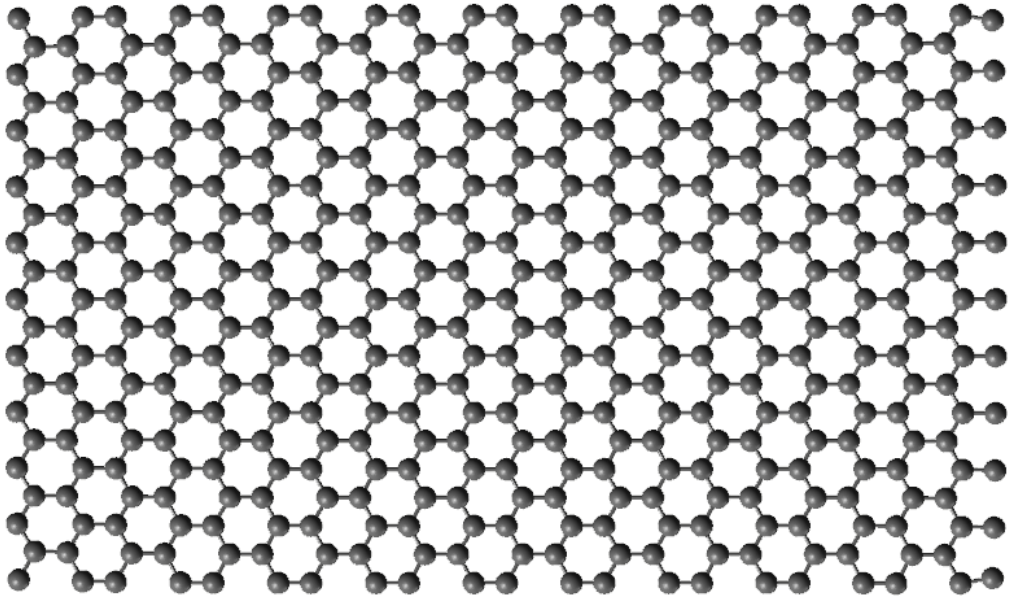
3.5 Individual commands

This section lists all LAMMPS commands alphabetically, with a separate listing below of styles within certain commands. The previous section lists the same commands, grouped by category. Note that some style options for some commands are part of specific LAMMPS packages, which means they cannot be used unless the package was included when LAMMPS was built. Not all packages are included in a default LAMMPS build. These dependencies are listed as Restrictions in the command's documentation.

angle_coeff	angle_style	atom_modify	atom_style	balance	bond_coeff
bond_style	boundary	box	change_box	clear	comm_modify
comm_style	compute	compute_modify	create_atoms	create_box	delete_atoms
delete_bonds	dielectric	dihedral_coeff	dihedral_style	dimension	displace_atoms
dump	dump image	dump_modify	dump movie	echo	fix
fix_modify	group	if	improper_coeff	improper_style	include
jump	kspace_modify	kspace_style	label	lattice	log
mass	minimize	min_modify	min_style	molecule	neb
neigh_modify	neighbor	newton	next	package	pair_coeff
pair_modify	pair_style	pair_write	partition	prd	print
processors	quit	read_data	read_dump	read_restart	region
replicate	rerun	reset_timestep	restart	run	run_style
set	shell	special_bonds	suffix	tad	temper
thermo	thermo_modify	thermo_style	timestep	uncompute	undump
unfix	units	variable	velocity	write_data	write_dump
write_restart					

Example 1: energy minimization

Generate a perfect graphene flake and found the configuration with minimal energy. Perform the same process for a defected graphene flake.



LAMMPS code

Example 1: energy minimization

```
1   # Input for energy minimization
2   #------------------------INITIALIZATION----
3   units           metal
4   boundary        p p p
5
6   atom_style      atomic
```

Options:

- x,y,z = *p* or *s* or *f* or *m*, one or two letters

```
p is periodic
f is non-periodic and fixed
```

Options:

- style = *angle* or *atomic* or *body* or *bond* or *charge*

angle	bonds and angles
atomic	only the default values
body	mass, inertia moments, quaternion, angular momentum
bond	bonds
charge	charge

Options:

- style = *lj* or *real* or *metal* or *si* or *cgs*

"units metal":

- mass = grams/mole
- distance = Angstroms
- time = picoseconds
- energy = eV
- velocity = Angstroms/picosecond
- force = eV/Angstrom
- torque = eV
- temperature = Kelvin
- pressure = bars
- dynamic viscosity = Poise
- charge = multiple of electron charge
- dipole = charge*Angstroms
- electric field = volts/Angstrom
- density = gram/cm^dim

LAMMPS code

Example 1: energy minimization

```
 7
 8  #-----------------------ATOM DEFINITION----------------------------
 9  # Generating a graphene structure
10  lattice         custom 2.4595 a1 1  0  0 a2 0 1.73203 0 a3 0.0 0.0 4 &
11                  basis 0 0 0 basis 0.5 0.16666666666666666 0  basis 0.5 0.5 0 basis 0 0.6666666666666666 0
```

`lattice style scale keyword values`

Options:

- style = *none* or *sc* or *bcc* or *fcc* or *hcp*
- zero or more keyword/value pairs may be appended
- keyword = *origin* or *orient* or *spacing* or *a1* or *a2* or *a3* or *basis*

```
13  # C atoms region
14  region          grap block 0 10 0 10 -0.5 0.5
15
16  # Simulation box size
17  region          boundary block -5 15 -5 15 -5 5
18
19  # Combine regions
20  region          whole union 2 grap boundary
21
22  # Create viewing box
23  create_box      1 boundary
```

`region ID style args keyword arg`

Options:

- ID = user-assigned name for the region
- style = *delete* or *block* or *cone* or *cylinder* or *sphere* or *union* or *intersect*

LAMMPS code

Example 1: energy minimization

```
 7
 8  #----------------------ATOM DEFINITION---------------------------
 9  # Generating a graphene structure
10  lattice         custom 2.4595 a1 1  0  0 a2 0 1.73203 0 a3 0.0 0.0 4 &
11                  basis 0 0 0 basis 0.5 0.16666666666666666 0  basis 0.5 0.5 0 basis 0 0.6666666666666666 0
```

`lattice style scale keyword values`

Options:

- style = *none* or *sc* or *bcc* or *fcc* or *hcp*
- zero or more keyword/value pairs may be appended
- keyword = *origin* or *orient* or *spacing* or *a1* or *a2* or *a3* or *basis*

```
13  # C atoms region
14  region          grap block 0 10 0 10 -0.5 0.5
15
16  # Simulation box size
17  region          boundary block -5 15 -5 15 -5 5
18
19  # Combine regions
20  region          whole union 2 grap boundary
21
22  # Create viewing box
23  create_box      1 boundary
```

`create_box N region-ID`

Options:

- N = # of atom types to use in this simulation
- region-ID = ID of region to use as simulation domain

LAMMPS code

Example 1: energy minimization

```
25  # Creating C atoms
26  create_atoms     1 region grap
27  mass             1 12
28  group            sample region grap
29
```

```
30  #-----------------------FORCE FIELDS-----
31  # Interaction potential for carbon atoms
32  pair_style       tersoff
33  pair_coeff       * * SiC_1994.tersoff C
34
35  neighbor         2.0 bin
36  neigh_modify     delay 0
```

`create_atoms type style args`

Options:

- type = atom type (1-Ntypes) of atoms to create
- style = *box* or *region* or *single* or *random*

`pair_style style args`

Options:

- style = one of the styles from the list below
- args = arguments used by a particular style

pair_style eam

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}(r_{ij})$$

pair_style coul/cut

$$E = \frac{Cq_iq_j}{\epsilon r} \qquad r < r_c$$

Example 1: energy minimization

```
25  # Creating C atoms
26  create_atoms     1 region grap
27  mass             1 12
28  group            sample region grap
29
```

`create_atoms type style args`

Options:

- type = atom type (1-Ntypes) of atoms to create
- style = *box* or *region* or *single* or *random*

```
30  #------------------------FORCE FIELDS-----
31  # Interaction potential for carbon atoms
32  pair_style       tersoff
33  pair_coeff       * * SiC_1994.tersoff C
34
35  neighbor         2.0 bin
36  neigh_modify     delay 0
```

`pair_coeff I J args`

Options:

- I,J = atom types (see asterisk form below)
- args = coefficients for one or more pairs of atom types

LAMMPS code

Example 1: energy minimization

```
38  #------------------------SIMULATION PROCESS-------------------------------
39  # Initial velocities at a given temperature
40  velocity        all create 100 458273253 dist gaussian
41
42  # Timestep to make the integration of the motion equation
43  timestep        0.001
44
45  # Parameters to print out on the screen and log.lammps file
46  thermo_style    custom step temp etotal vol lx ly lz press pxx pyy pzz cpu
47  thermo          1000
48
```

`thermo_style style args`

Options:

- style = *one* or *multi* or *custom*
- args = list of arguments for a particular style

`thermo N`

Options:

- N = output thermodynamics every N timesteps

LAMMPS code

Example 1: energy minimization

```
49  # Saving atomic coordinates
50  dump            1 all xyz 1000 dump-*.xyz
51  dump_modify     1 element C
52
53  # Energy minimization parameters
54  min_style       cg
55  minimize        1.0e-10 1.0e-12 100000 10000
56
57  #-----SIMULATION DONE-------
58  print           "Simulation complete"
```

`dump ID group-ID style N file args`

Options:

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be dumped
- style = *atom* or *atom/mpiio* or *cfg* or *dcd* or *xtc* or *xyz*
- N = dump every this many timesteps
- file = name of file to write dump info to
- args = list of arguments for a particular style

`min_style style`

Options:

- style = *cg* or *hftn* or *sd* or *quickmin* or *fire*

`minimize etol ftol maxiter maxeval`

Options:

- etol = stopping tolerance for energy (unitless)
- ftol = stopping tolerance for force (force units)
- maxiter = max iterations of minimizer
- maxeval = max number of force/energy evaluations

RUN LAMMPS: Open a console and write,

$ **lmp < lammps.inp**

LAMMPS code

XYZ file

Number of atoms

48

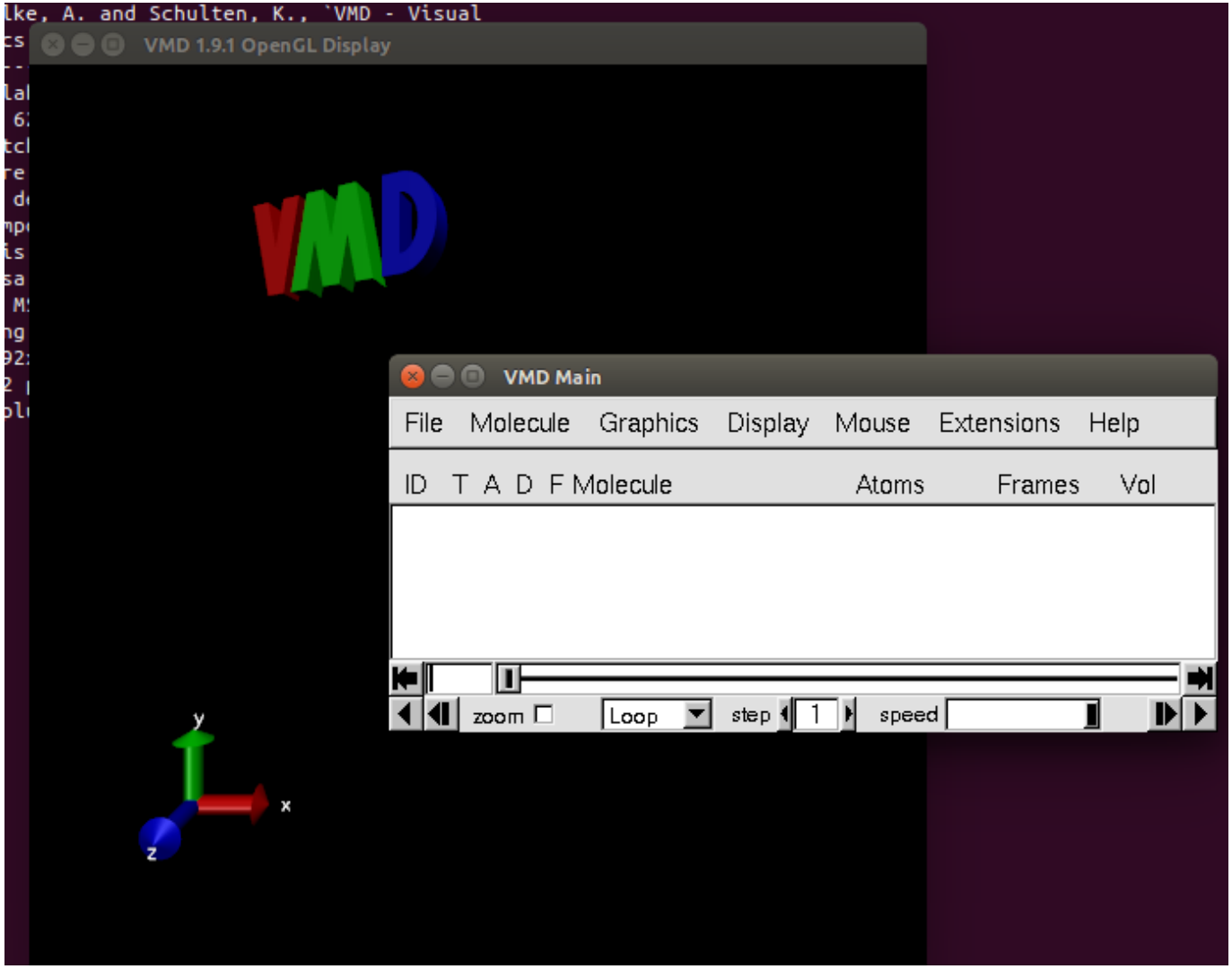
Atomic positions (x,y,z)

Chemical symbol of the atoms

C	0.00000000	17.09466934	-4.03419018
C	0.00000000	1.45693004	-6.26033020
C	0.00000000	2.33809996	-7.37733984
C	0.00000000	3.75167990	-7.17118979
C	0.00000000	4.30586004	-5.85873985
C	0.00000000	1.12878001	-3.83152008
C	0.00000000	2.01055002	-4.94802999
C	0.00000000	3.42429996	-4.74241018
C	0.00000000	3.97836995	-3.43022990
C	0.00000000	0.80035001	-1.40403998
C	0.00000000	1.68262994	-2.51986003
C	0.00000000	3.09647989	-2.31424999
C	0.00000000	3.65089989	-1.00232995
C	0.00000000	5.71954012	-5.65229988
C	0.00000000	6.60097980	-6.76849985

LAMMPS code

VMD Visualizer



Open a console and write: **VMD**.

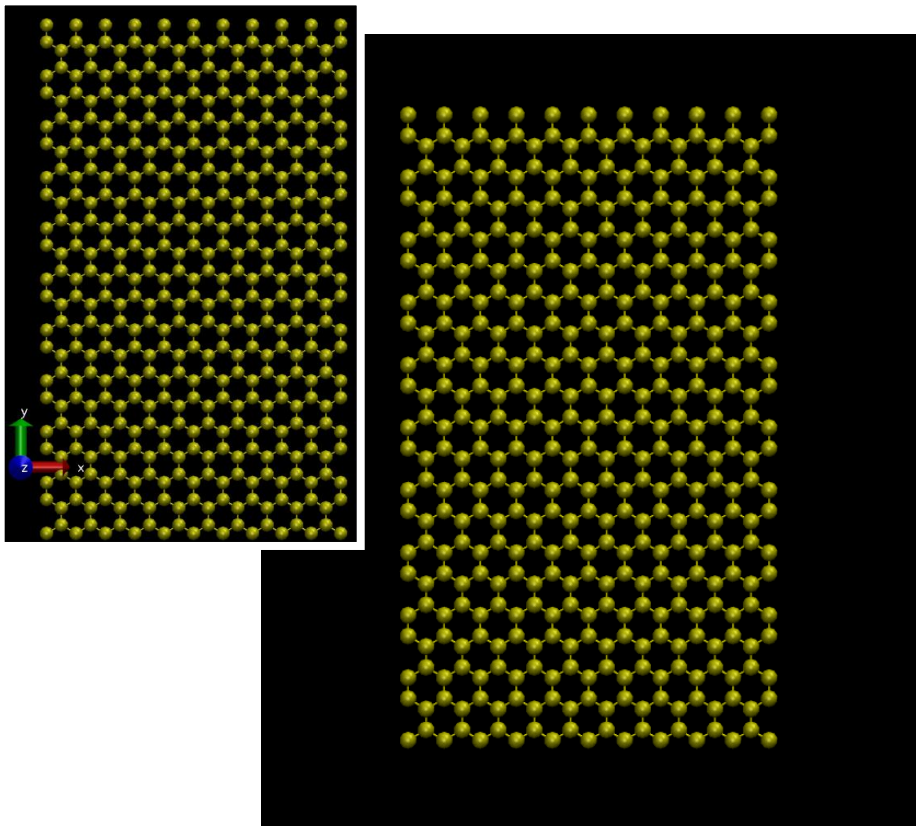
It is also possible to do:

>$ vmd file.xyz

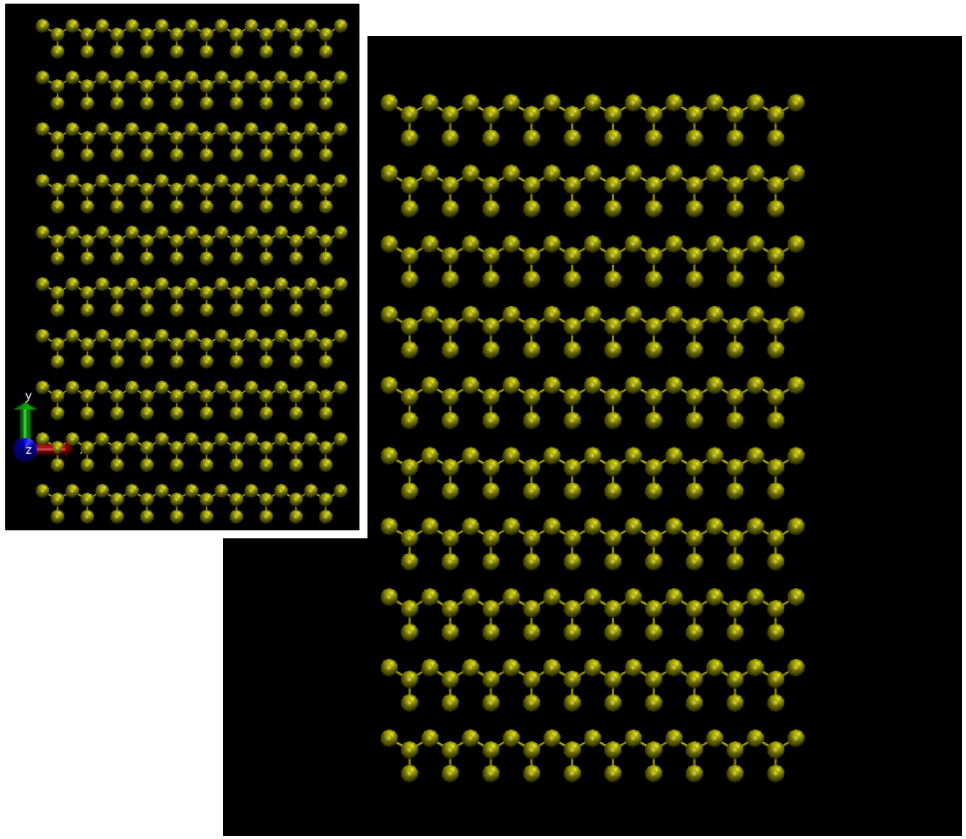
Example 1: energy minimization

Generate a perfect graphene flake and found the configuration with minimal energy. Perform the same process for a defected graphene flake.

Without defects



With defects



Example 2: thermal relaxation

Generate a perfect silver bulk structure (fcc structure, L=2.5 nm). Then, perform the following tasks:

- Thermal relaxation at 300 K for 20 ps and calculate the total energy of the system.
- Make a plot of the temperature dependence of the total energy. Temperature range: 300 – 1500 K and simulation time = 500 ps.

LAMMPS code

Example 2: thermal relaxation

```
1   # Input for thermal relaxation
2   #------------------------INITIALIZATION-----------------------------
3   units           metal
4   boundary        p p p
5
6   atom_style      atomic
7
8   #----------------------ATOM DEFINITION-----------------------------
9   # Generating a fcc structure
10  lattice         fcc 4.09 origin 0 0 0
11
12  # Ag atoms region
13  region          silver block 2 8 2 8 -3 3
14
15  # Simulation box size
16  region          boundary block 2 8 2 8 -3 3
17
18  # Combine regions
19  region          whole union 2 silver boundary
20
21  # Create viewing box
22  create_box      1 boundary
23
24  # Creating Ag atoms
25  create_atoms    1 region silver
26  mass            1 107.87
27  group           sample region silver
28
```

LAMMPS code

Example 2: thermal relaxation

```
29  #------------------------FORCE FIELDS-----------------------------
30  # Interaction potential for silver atoms
31  pair_style      eam
32  pair_coeff      * * Ag_u3.eam
33
34  neighbor        2.0 bin
35  neigh_modify    delay 0
36
37  #------------------------SIMULATION PROCESS-----------------------------
38  # Initial velocities at a given temperature
39  velocity        all create 300 458273253 dist gaussian
40
41  # Nose-Hoover thermostat
42  fix             nvt1 all nvt temp 300.0 500.0 0.1
43
44  # Timestep to make the integration of the motion equation
45  timestep        0.001
46
47  # Parameters to print out on the screen and log.lammps file
48  thermo_style    custom step temp etotal vol lx ly lz press pxx pyy pzz cpu
49  thermo          1000
50
```

We use this command to control the temperature of the system under a NVT ensemble.

fix ID ID-group nvt temp Tstart TFinal TDamp

LAMMPS code

Example 2: thermal relaxation

```
51  # Saving atomic coordinates
52  dump            1 all xyz 1000 dump-*.xyz
53  dump_modify     1 element Ag
54
55  # Saving data to analyze
56  variable        Temperature equal temp
57  variable        TEnergy equal etotal
58  variable        KEnergy equal ke
59
60  fix             temp_out all ave/time 100 10 1000 v_Temperature v_TEnergy v_KEnergy file data.out
61
62  # Number of simulation steps
63  run             20000
64
65  #-----SIMULATION DONE-------
66  print         "Simulation complete"
```

We define new variables that we want to analyze and save them in the file **"data.out"**. The data is saved over an specific range of time (average). In this case we take the average among the values corresponding to 100, 200, 300, 400, ……, 1000 **timesteps**.

This command defines the simulation time:

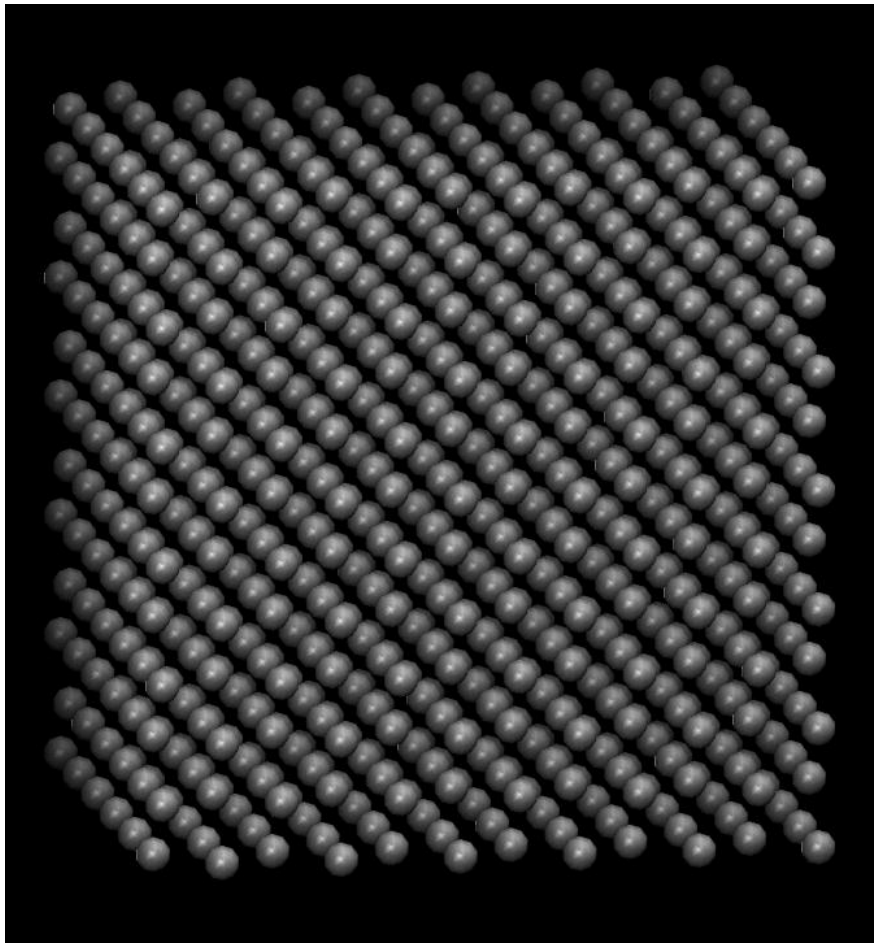
simulation time = timestep*#run

Example 2: thermal relaxation

Generate a perfect silver bulk structure (fcc structure, L=2.5 nm). Then, perform the following tasks:

- Thermal relaxation at 300 K for 20 ps and calculate the total energy of the system.

Total energy = -2396.25 eV



LAMMPS code

Example 2: thermal relaxation

Generate a perfect silver bulk structure (fcc structure, L=2.5 nm). Then, perform the following tasks:

- ❑ Thermal relaxation at 300 K for 20 ps and calculate the total energy of the system.
- ❑ Make a plot of the temperature dependence of the total energy. Temperature range: 300 – 1500 K and simulation time = 500 ps.