Computational Nanoscience

NSE C242 & Phys C203

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Lecture 5:

In-Class Simulation:

MD of Carbon Nanostructures

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LAMMPS-MD Simulations

Today we'll be doing simulations in class using a code called "LAMMPS" - again, brought to you via a brilliantly intuitive web interface on the nanohub.

Before we start, what is LAMMPS?

LAMMPS is a molecular dynamics code developed at Sandia NL.

LAMMPS = Large-scale Atomic/Molecular Massively Parallel Simulator.

It is freely available for download, and comes with a variety of interatomic potentials built-in.

See the LAMMPS homepage at http://lammps.sandia.gov.

We will be using periodic boundary conditions for all of our simulations today.

LAMMPS-MD Simulator

Today, we will be exploring carbon based structures such as nanotubes, graphene, fullerenes, and diamond.

This means we need a potential to describe the carbon-carbon interaction. We're going to use something called a Tersoff Potential (named after it's creator Jerry Tersoff). See J. Tersoff, Phys Rev B, 37, 6991 (1988) and many thereafter.

The salient feature of the Tersoff potential is that it is a bond order potential, which is a high-fallutin' way of saying that the interaction looks like this:

$$V_{ij}\left(r_{ij}\right) = V_{rep}\left(r_{ij}\right) + b_{ij} V_{att}\left(r_{ij}\right)$$

$$b_{ij} = b_{ij}\left(g_{ij}\right) \quad ; \quad g_{ij} = \sum_{k} f_c(r_{ik}) g\left(\theta_{jik}\right) f\left(r_{ij} - r_{ik}\right)$$

b_{ij} is the "bond-order" and g_{ij} is the "coordination". This last terms serves to weaken the bond between atoms i and j thanks to the presence of other neighboring atoms k.

Basically, it's a decent short-range potential that depends on local coordination and on bond angles. Thus, it can describe the different bonding states of an atom (for instance, sp^2 vs. sp^3).

Tersoff potentials exist for carbon, silicon, silicon-carbon, germanium. They have been extended to a wide variety of other systems (e.g. Tersoff-Brenner potential for hydrocarbons, etc).

MD at Constant Temperature

One difference in LAMMPS from our simpler, LJ-MD simulations, is that we now have the option of applying a thermostat or minimizing the energy.

What does a thermostat do?

Very simply, it couples the simulation box to an external "heat bath."

A number of approaches have been developed to do this, e.g.,

- velocity rescaling (a bit ad-hoc, with many different implementations)
- Andersen thermostat (JCP **72**, 2384 (1980))
- Nose-Hoover thermostat (JCP **81**, 511 (1984) and PRA **31**, 1695 (1985))

First Task: Energy Minimization

Let's start with some simple minimization examples on the fullerenes C60, C70, C84, and C100.

Do a geometry optimization run for each of these. Now do a geometry optimization for a sheet of graphene as well.

Be sure to look at the output, and assure yourself that the energy has, indeed, converged. LAMMPS has standard defaults that tell it when the convergence is acceptable (you could adjust these for yourself if you wanted).

What are the relative binding energies per atom for each of the structures? Is this what you would expect?

Are any of these the lowest energy structures for the model potential we're using? What else might you consider?

Second Task:Young's Modulus

Choose a carbon nanotube with no defects, and optimize its structure.

Now, compute the Young's modulus of your nanotube at 0K by computing the energy for different axial strains.

E=stress/strain=[force/area]/[(change in length)/length]

How might one go about doing this?

Is the modulus larger or smaller than the Young's modulus of Steel ($200X10^9$ N/m^2)?

Find a value from the literature and compare with that.

Now choose the same carbon nanotube, but with a Stone-Wales defect present. Repeat the exercise. Does the defect change the Young's Modulus?

Third Task: MD at Constant Temperature

Now we'll explore the NVT ensemble using the Nose-Hoover thermostat.

Stick with your defect free nanotube from the previous exercise.

Determine what timestep is necessary to sample the system appropriately at 300K, 1000K, and 2000K.

How can you tell what a good timestep is?

Does the timestep change for the different temperatures?

Fourth Task: Now for Some NVE …

Now we'll explore the NVE ensemble.

Your task is to compute the Young's Modulus for a (defect-free and defective) carbon nanotube at 1000K.

What are some considerations regarding the average energy of the system at various strain rates? (There are now error bars on your calculation of the energy!)