

AE/AM/CE/ME 102b Homework 4

Mechanics of Structures and Solids - Winter 2012

Due: Tuesday, February 7, 2012, 9:00am in class

Office Hours:

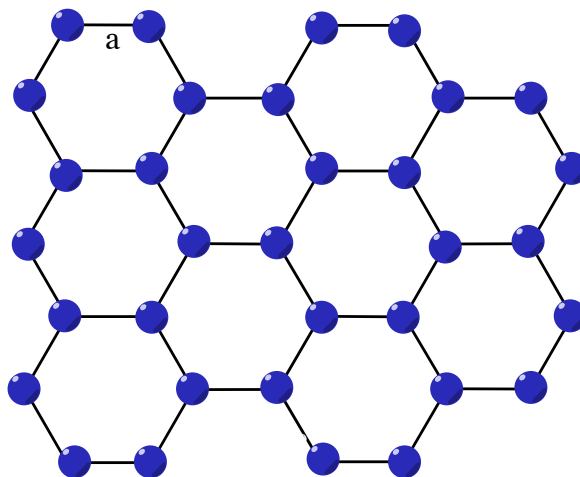
Kaushik Bhattacharya (bhatta@caltech.edu) - By appointment

Ha Giang (hagiang@caltech.edu): M 5 - 6pm, SFL Multimedia Conference Room

Xin (Cindy) Wang (xxwang@caltech.edu): F 4:30 - 5:30pm, SFL Multimedia Conference Room

Problem 1

Carbon nanotubes can be thought of as a rolled-up graphene sheet. A graphene sheet is a two-dimensional crystal of carbon atoms with the atoms arranged in a regular hexagonal arrangement as shown.



- Show that this regular hexagonal arrangement does not form a Bravais lattice.
- Show that this regular hexagonal arrangement can be thought of as a two-lattice, i.e. as a superposition of two identical Bravais lattices that are translated from each other.
- The Tersoff-Brenner potential is often used as a model for carbon. Since each atom has an identical environment up to rotations, it is possible to define the energy per atom. Find the energy per atom limiting yourself to nearest neighbor interactions.
- Find the equilibrium inter-atomic spacing a , limiting yourself to nearest neighbor interactions. How does it compare with the observed spacing on 0.1415 nm?

Tersoff-Brenner Potential

Brenner (1990) established an iteratomic potential for carbon from Tersoff (1988) formalism as

$$V(r_{ij}) = V_R(r_{ij}) - B_{ij}V_A(r_{ij}) \quad (1)$$

for atoms i and j , where r_{ij} is the distance between atoms i and j , V_R and V_A are the repulsive and attractive pair terms (i.e., depending only on r_{ij}) and are given by

$$V_R(r) = \frac{D^{(e)}}{S-1} e^{-\sqrt{(2S)\beta}(r-R^{(e)})} f_c(r), \quad (2)$$

$$V_A(r) = \frac{D^{(e)}S}{S-1} e^{-\sqrt{(2/S)\beta}(r-R^{(e)})} f_c(r); \quad (3)$$

the parameters $D^{(e)}$, S , β , and $R^{(e)}$ are determined from the known physical properties of carbon, graphite, and diamond, and are given at the end of this section; the function f_c is merely a smooth cutoff function to limit the range of the potential, and is given by

$$f_c(r) = \begin{cases} 1 & r < R^{(1)} \\ \frac{1}{2} \left(1 + \cos \frac{\pi(r-R^{(1)})}{R^{(2)}-R^{(1)}} \right) & R^{(1)} < r < R^{(2)} \\ 0 & r > R^{(2)} \end{cases} \quad (4)$$

which is continuous and has a cutoff of $R^{(2)} = 0.2$ nm and $R^{(1)} = 0.17$ nm to include only the first-neighbor shell for carbon.

The parameter B_{ij} in equation (1) represents a multi-body coupling between the bond from atom i to atom j and the local environment of atom i , and is given by

$$B_{ij} = \left(1 + \sum_{k(\neq i,j)} G(\theta_{ijk}) f_c(r_{ik}) \right)^{(-\delta)}, \quad (5)$$

where k represents atoms other than i and j , r_{ik} is the distance between atoms i and k , f_c is the cutoff function in equation (4), θ_{ijk} is the angle between bonds $i-j$ and $i-k$, and the function G is given by

$$G(\theta) = a_0 \left(1 + \frac{c_0^2}{d_0^2} - \frac{c_0^2}{d_0^2 + (1 + \cos \theta)^2} \right) \quad (6)$$

The parameters $D^{(e)}$, S , β , and $R^{(e)}$ in equation (2) and (3), δ in equation (5), and a_0 , c_0 , and d_0 in equation (6) have been determined by Brenner (1990) to fit the binding energy and lattice constants of graphite, diamond, simple cubic and face-centered-cubic structures for pure carbon, as well as the vacancy formation energy for diamond and graphite as

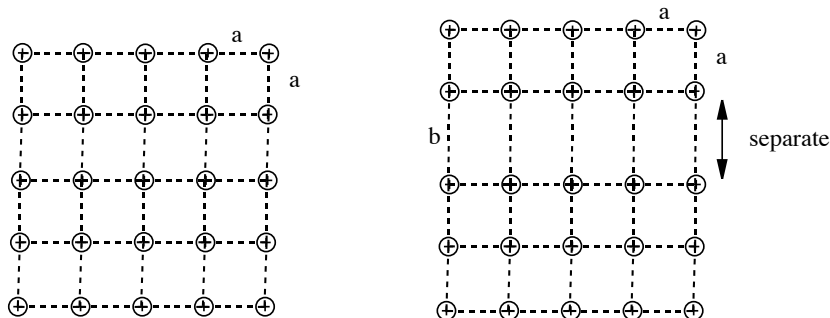
$$\begin{aligned} D^{(e)} &= 6.000 \text{ eV}, & S &= 1.22, & \beta &= 21 \text{ nm}^{-1}, & R^{(e)} &= 0.1390 \text{ nm}, \\ \delta &= 0.50000, & a_0 &= 0.00020813, & c_0 &= 330, & d_0 &= 3.5. \end{aligned} \quad (7)$$

Problem 2

Consider a simple 3D cubic lattice with atomic spacing a , and interacting with a Leonard Jones pair potential limiting to the nearest neighbor interaction:

$$\psi(r) = V_0 \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad V_0 = 0.08 \text{ eV/atom}, \quad \sigma = 4 \text{ \AA} \quad (8)$$

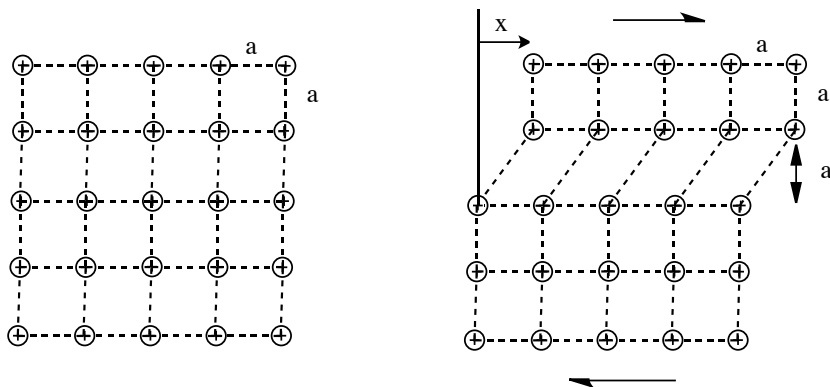
Assuming the atomic spacing a minimizes the energy per atom in the reference lattice.



Suppose we separate the lattice into two parts as shown above, find the excess energy of the lattice per column of atoms as a function of b . Find the excess energy per unit reference area. Compare this with a typical observed fracture energy of 1 J/cm^2 . Comment on your answer.

Note: excess energy is the energy difference between a lattice with separation and a lattice without one; nearest neighbor interaction means interaction with six atoms here; $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$; $1 \text{ \AA} = 10^{-10} \text{ m}$.

Problem 3



Find the excess energy of the lattice per column of atoms as a function of x if shear stress is applied to the lattice in Problem 2 as shown in the figure above. Compute the shear force as a function of x and compare to the sinusoidal shear force $\tau = k \sin \frac{2\pi x}{a}$ that we used in class.

Note: nearest neighbor interaction means interaction with six atoms here, and the nearest neighbors changes.