

AE/AM/CE/ME 102b Homework 3

Mechanics of Structures and Solids - Winter 2012

Due: January 31, 2012 9:00am in class

Office Hours:

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

Ha Giang (hagiang@caltech.edu) - Monday 5pm - 6pm, SFL Multimedia Conference Room (3rd floor)

Xin (Cindy) Wang (xxwang@caltech.edu) - Friday 4:30pm - 5:30pm, SFL Multimedia Conference Room (3rd floor)

1. Consider a face centered cubic lattice shown in Figure 1. Suppose its atoms interact through a Lennard-Jones potential

$$\Psi(r) = V_0 \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

- a) Calculate the energy per atom, assuming only first, second and third neighbor interactions.
 - b) Find the lattice parameter a that minimizes the energy per atom.
 - c) Given that $a = 6.13 \text{ \AA}$ and cohesive energy (energy per atom at the correct lattice parameter) = -0.17 eV/atom (corresponding to Xenon), find the constants V_0 and σ .
2. For the values of V_0 and σ determined in 1 c), find the lattice parameter and cohesive energy assuming the lattice structure to be body-centered-cubic as shown in Figure 2 (limit yourself to first, second and third neighbor interactions only).
 3. Consider a 2-dimensional Bravais lattice. Show that the point group or the symmetry group is

$$\begin{aligned} P(e_i) &= \{R : Re_i = \mu_i^j e_j\} \\ &= \begin{cases} \{R_0, R_{\frac{\pi}{3}}, R_{\frac{2\pi}{3}}, R_{\pi}, R_{\frac{4\pi}{3}}, R_{\frac{5\pi}{3}}\} & \text{if } |e_1| = |e_2|, \frac{e_1 \cdot e_2}{|e_1||e_2|} = \frac{1}{2} \text{ (a triangular lattice)} \\ \{R_0, R_{\frac{\pi}{2}}, R_{\pi}, R_{\frac{3\pi}{2}}\} & \text{if } |e_1| = |e_2|, \frac{e_1 \cdot e_2}{|e_1||e_2|} = 0 \text{ (a square lattice)} \\ \{R_0, R_{\pi}\} & \text{otherwise} \end{cases} \end{aligned}$$

where R_θ is a rotation by an angle θ .

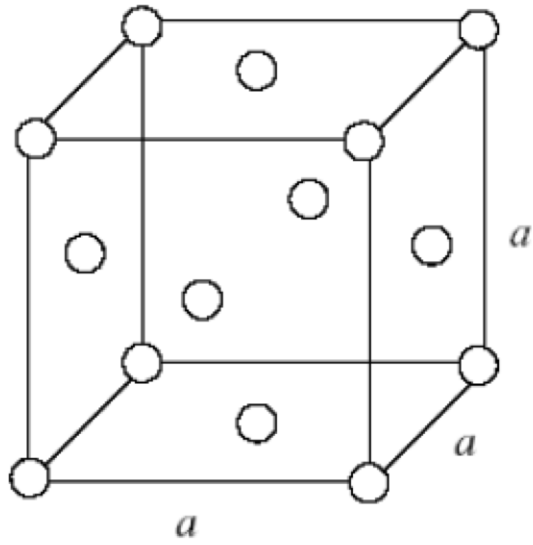


Figure 1: Face-centered-cubic lattice for problem 1

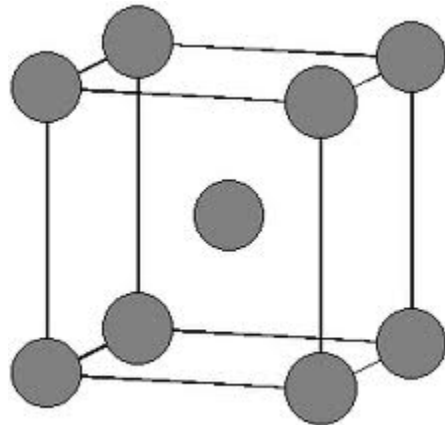


Figure 2: Body-centered-cubic lattice for problem 2