AE/AM/CE/ME 102b Homework 3 Solutions

Mechanics of Structures and Solids - Winter 2012

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

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

a) Calculate the energy per atom, assuming only first, second and third neighbor interactions.

Solution:

In an FCC lattice, for a given atom, it has 12 nearest neighbors at a distance $\frac{a}{\sqrt{2}}$ away; 6 second nearest atoms at a distance a away; 24 third nearest atoms at a distance $\frac{\sqrt{3}a}{\sqrt{2}}$ away. The total energy per atom counting only up to third nearest neighbors is:

$$\begin{aligned}
E_{\text{atom}} &= \frac{1}{2}\sum_{i=1}^{3} N_i * \Psi(r_i) \\
&= \frac{1}{2}\{12V_0[(\frac{\sqrt{2}\sigma}{a})^{12} - (\frac{\sqrt{2}\sigma}{a})^6] + [6V_0[(\frac{\sigma}{a})^{12} - (\frac{\sigma}{a})^6] + [24V_0[(\frac{\sqrt{2}\sigma}{\sqrt{3}a})^{12} - (\frac{\sqrt{2}\sigma}{\sqrt{3}a})^6]\} \\
&= \frac{1}{2}V_0\{776\frac{26}{243}(\frac{\sigma}{a})^{12} - 109\frac{1}{9}(\frac{\sigma}{a})^6\}
\end{aligned}$$

b) Find the lattice parameter a that minimizes the energy per atom.

Solution:

$$E_{\text{atom}}(a) = \frac{1}{2}V_0\{776\frac{26}{243}(\frac{\sigma}{a})^{12} - 109\frac{1}{9}(\frac{\sigma}{a})^6\}$$

We need to minimize the energy with respect to lattice parameter a:

$$\begin{aligned}
\frac{dE_{\text{atom}(a)}}{da} &= \frac{1}{2}V_0\{-9313\frac{23}{81}(\frac{\sigma^{12}}{a^{13}}) + 654\frac{2}{3}(\frac{\sigma^6}{a^7})\} = 0 \quad (1)\\
\implies & \frac{9313\frac{23}{81}}{654\frac{2}{3}}\sigma^6 = a^6 \quad (2)\\
\implies & a = 1.5566\sigma \quad (3)
\end{aligned}$$

We need to take the second derivative with respect to a to ensure that we have a minimum:

$$\begin{aligned}
\frac{d^2E}{da^2} &= \frac{V_0}{2}\{\frac{121072.67\sigma^{12}}{a^{14}} - \frac{4582.69\sigma^6}{a^8}\} \quad (4)\\
&= \frac{V_0}{2a^2}\{\frac{121072.67}{1.5567^{12}} - \frac{4582.69}{1.5567^6}\} \quad (5)
\end{aligned}$$

We see that if V_0 is positive, then we have a minimum.

c) Given that $a = 6.13$ Å 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.

Solution:

$a = 6.13$ Å implies that

$$\begin{aligned}
6.13\text{Å} &= 1.5566\sigma\\
&\implies \sigma = 3.93\text{Å}
\end{aligned}$$

From a)

$$\begin{aligned}
E_{\text{atom}}(a) &= \frac{1}{2}V_0\{776\frac{26}{243}(\frac{\sigma}{a})^{12} - 109\frac{1}{9}(\frac{\sigma}{a})^6\}\\
&= \frac{1}{2}V_0\{776\frac{26}{243}(\frac{1}{1.5566})^{12} - 109\frac{1}{9}(\frac{1}{1.5566})^6\}\\
&\implies V_0 = 0.08866\text{eV}
\end{aligned}$$

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).

Solution:

In an BCC lattice, for a given atom, it has 8 nearest neighbors at a distance $\frac{\sqrt{3}a}{2}$ away; 6 second nearest atoms at a distance a away; 12 third nearest atoms at a distance $\sqrt{2}a$ away. The total energy per atom counting only up to third nearest neighbors is:

$$\begin{aligned}
E_{\text{atom}} &= \frac{1}{2}\sum_{i=1}^{3} N_i * \Psi(r_i)\\
&= \frac{1}{2}\{8V_0[(\frac{2\sigma}{\sqrt{3}a})^{12} - (\frac{2\sigma}{\sqrt{3}a})^6] + [6V_0[(\frac{\sigma}{a})^{12} - (\frac{\sigma}{a})^6] + [12V_0[(\frac{\sigma}{\sqrt{2}a})^{12} - (\frac{\sigma}{\sqrt{2}a})^6]\}\\
&= \frac{1}{2}V_0\{25.57(\frac{\sigma}{a})^{12} - 13.23(\frac{\sigma}{a})^6\}
\end{aligned}$$

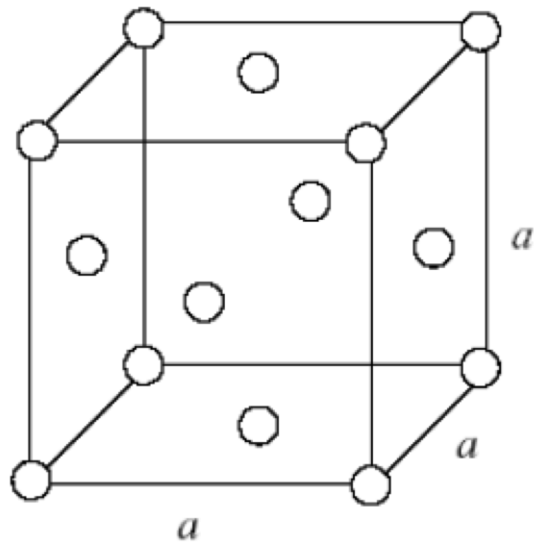

Figure 1: Face-centered-cubic lattice for problem 1

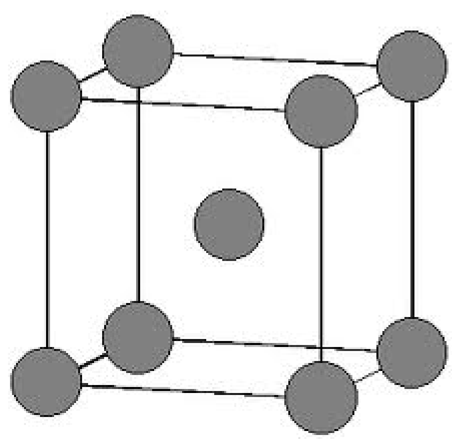

Figure 2: Body-centered-cubic lattice for problem 2

We need to minimize the energy with respect to lattice parameter a:

$$\frac{dE_{\text{atom}(a)}}{da} = \frac{1}{2}V_0\{-306.82(\frac{\sigma^{12}}{a^{13}}) + 79.39(\frac{\sigma^6}{a^7})\} = 0 \quad (6)$$

$$\implies \frac{306.82}{79.39}\sigma^6 = a^6 \quad (7)$$

$$\implies a = 1.253\sigma \quad (8)$$

Taking the second derivative with respect to a to show that we have a minimum:

$$\frac{d^2E}{da^2} = \frac{V_0}{2}\{\frac{3988.7\sigma^{12}}{a^{14}} - \frac{555.73\sigma^6}{a^8}\} \quad (9)$$

$$= \frac{V_0}{2a^2}\{\frac{3988.7}{1.253^{12}} - \frac{555.73}{1.253^6}\} \quad (10)$$

$$\implies \frac{d^2E}{da^2} > 0 \quad (11)$$

Since V_0 is positive from problem 1, then we have a minimum;

Using V_0 and σ from problem 1:

$$a = 1.253 * 3.93\mathring{A} = 4.924\mathring{A}$$

$$E_{\text{atom}} = \frac{1}{2}V_0\{25.57(\frac{1}{1.253})^{12} - 13.23(\frac{1}{1.253})^6\}$$

$$\implies E_{\text{atom}} = -0.1518\text{eV}$$

3. Consider a 2-dimensional Bravais lattice. Show that the point group or the symmetry group is

$$P(e_i) = \{R : Re_i = \mu_i^j e_j\}$$

$$= \begin{cases} \{R_0, R_{\frac{\pi}{3}}, R_{\frac{2\pi}{3}}, R_\pi, R_{\frac{4\pi}{3}}, R_{\frac{5\pi}{3}}\} & \text{if } |e_1| = |e_2|, \frac{e_1 \cdot e_2}{|e_1||e_2|} = \frac{1}{2} \text{ (a triangular lattice)} \\ \{R_0, R_{\frac{\pi}{2}}, R_\pi, R_{\frac{3\pi}{2}}\} & \text{if } |e_1| = |e_2|, \frac{e_1 \cdot e_2}{|e_1||e_2|} = 0 \text{ (a square lattice)} \\ \{R_0, R_\pi\} & \text{otherwise} \end{cases}$$

where R_θ is a rotation by an angle θ.

Solution:

An instance of rotational tensor Q in 2D is:

$$Q = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \quad (12)$$

Since the trace is one of the invariant quantities of all rotational tensors, we can conclude that all the trace of the rotational tensors in 2D take the form of:

$$\text{Tr}(Q) = 2\cos(\theta)$$

Since we know that transformations that map between lattice vectors must be take integer values. We can find all the angle θ such that we have an integer trace for Q:

$$\theta = 0, \frac{\pi}{3}, \frac{\pi}{2}, \frac{3\pi}{2}, 2\pi$$

Now we can proceed to find all possible rotational point groups that can contain any of the above angles. Remember the 3 properties of a point group are:

(a) Contains a 0 transformation.

(b) Contains an inverse transformation for each member of the group.

(c) Closed under the operation $*$.

Restricting the angle θ to be between $\{0, 2\pi\}$, we find that the following point groups are available:

1. $\{0\}$
2. $\{0, \pi\}$
3. $\{0, \frac{\pi}{3}, \frac{2\pi}{3}, \pi, \frac{4\pi}{3}, \frac{5\pi}{3}\}$
4. $\{0, \frac{2\pi}{3}, \frac{4\pi}{3}\}$
5. $\{0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}\}$

We see that the triangular lattice contains the angle $\theta = \frac{\pi}{3}$, hence it must have the symmetry group: $\{0, \frac{\pi}{3}, \frac{2\pi}{3}, \pi, \frac{4\pi}{3}, \frac{5\pi}{3}\}$. Similarly the Square lattice contains the angle $\theta = \frac{\pi}{2}$, hence it must have the symmetry group: $\{0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}\}$. All other lattice, there does not exist any symmetry between lattice vectors e_1 and e_2, hence, we can only rotate the lattice vectors by $\{0, \pi\}$ to recover the original bravais lattice.