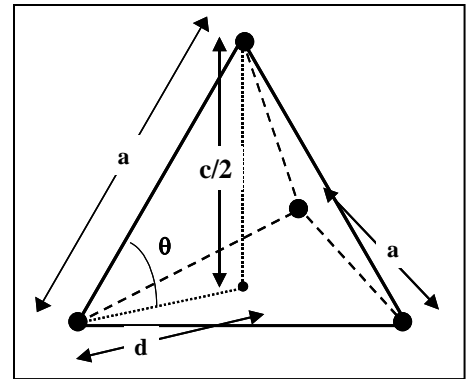


Homework 3 Solutions

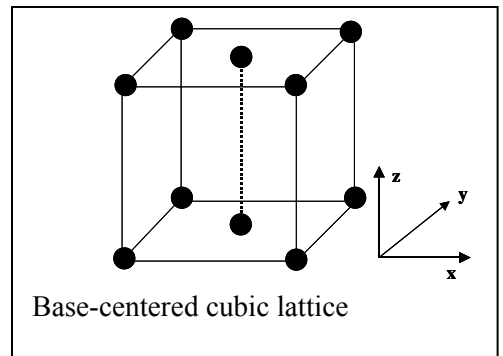
- The tetrahedral angles can be thought of as lying along the diagonals of a cube, the first one being the unit cube in the first octant of Cartesian space and represented by the unit vector $\mathbf{u}_1 = (3)^{-1/2} (\mathbf{x} + \mathbf{y} + \mathbf{z})$. We can form three unit vectors along other cube diagonals that are equiangular with this one by adding all permutations of two negations $\mathbf{u}_2 = (3)^{-1/2} (\mathbf{x} - \mathbf{y} - \mathbf{z})$, $\mathbf{u}_3 = (3)^{-1/2} (-\mathbf{x} + \mathbf{y} - \mathbf{z})$, and $\mathbf{u}_4 = (3)^{-1/2} (-\mathbf{x} - \mathbf{y} + \mathbf{z})$ (a little thought shows that adding just one negation, or three negations does not produce three other unique vectors). Then the angle between any two of these, θ , is given by the inner product definition: $\mathbf{u}_m \cdot \mathbf{u}_n = (1/3)(1 - 1 - 1) = \cos\theta$, or $\theta = \cos^{-1}(-1/3) = 70.5^\circ$.
- (a) by “ideal” hcp stacking, we mean the stacking of triangular lattices in a cannonball fashion. Since the cannonballs are identical, the center-to-center spacing between balls in the triangular lattice should be the same as the center-to-center nearest-neighbor spacing between layers. This means that the three points of a triangular unit cell and the point from the layer above them form the corners of a four-sided tetrahedron as shown in the figure to the right. The length of the hcp c axis is then half the height of the tetrahedron, and a is the length along the base. From trigonometry the distance d between a corner of the base and the center of the base is given by $a/(2d) = \cos(30^\circ)$. By the Pythagorean theorem, $(c/2)^2 = a^2 - d^2 = a^2 - a^2/(2\cos 30^\circ)^2$, or $c = 2a(1 - 1/3)^{1/2}$ or $c = (8/3)^{1/2} a$.



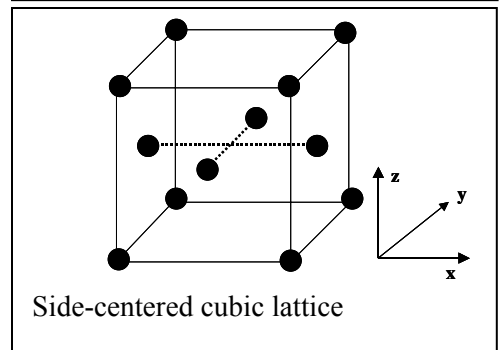
- The hcp lattice can be thought of as a simple hexagonal lattice with a single-atom basis (i.e., two atoms per primitive unit cell). So the density is given by $2/v$ where v is the primitive cell volume given by cA , where A is the area of the base of the tetrahedron. From trigonometry, $A = (3)^{1/2}a^2/2$ so the density is $\rho_{\text{hcp}} = 4/[(3)^{1/2}a^2c] = (2)^{1/2}/[(a_{\text{hcp}})^3]$. For the three common cubic lattices, simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc), we have densities $\rho_{\text{sc}} = 1/a^3$, $\rho_{\text{bcc}} = 2/a^3$ and $\rho_{\text{fcc}} = 4/a^3$ where a is the conventional cubic lattice constant. Assuming the densities stay fixed, we derive the following relationships: $a_{\text{hcp}} = [(2)^{1/2}]^{1/3} \cdot a_{\text{sc}} = [(2)^{1/2}/2]^{1/3} \cdot a_{\text{bcc}} = [(2)^{1/2}/4]^{1/3} \cdot a_{\text{fcc}}$.

3.

- Base-centered cubic (simple cubic plus one atom at the center of the top and bottom faces) is shown in the sketch at right. The arrangements of points around each lattice site is identical and the orientation is the same from point to point. So, yes, it is a Bravais lattice. Three primitive lattice vectors are: $\mathbf{a}_1 = (a/2)(\mathbf{x} + \mathbf{y})$, $\mathbf{a}_2 = (a/2)(\mathbf{x} + \mathbf{y})$, and $\mathbf{a}_3 = a \mathbf{z}$



- Side-centered cubic (simple cubic plus one atom at the center of each of the four sides) is shown in the sketch at right. This lattice has an orientation problem. Unlike the base-centered lattice, an atom in one of the side facets does not have the same environment as one in the bottom or top facets unless a rotation operation is also performed. So, no, it is not a Bravais lattice.



4.(a) We write the total potential energy of the linear chain in terms of the total number of atoms (ions)

$$2N: U(R) = N \left(\frac{ZA}{R^n} - \frac{\alpha q^2}{4\pi\epsilon_0 R} \right) = N \left(\frac{2A}{R^n} - \frac{2 \ln 2 q^2}{4\pi\epsilon_0 R} \right) = 2N \left(\frac{A}{R^n} - \frac{(\ln 2) q^2}{4\pi\epsilon_0 R} \right) \text{ for } Z=2, \text{ and for } \alpha =$$

$2 \ln 2$ – the Madelung constant for the chain. To find the equilibrium position R_0 , we differentiate with respect to R and set this to zero:

$$\left. \frac{dU}{dR} \right|_{R_0} = 0 = 2N \left(\frac{-nA}{R^{n+1}} + \frac{(\ln 2) q^2}{4\pi\epsilon_0 R^2} \right) \Big|_{R_0} \Rightarrow R_0^{-n} = \frac{q^2 \ln 2}{nAR_0 4\pi\epsilon_0}$$

Substitution back into $U(R)$ yields $U(R_0) = \frac{2N \ln 2 \cdot q^2}{4\pi\epsilon_0 R_0} \left(\frac{1}{n} - 1 \right)$ which becomes $\frac{-N \ln 2 \cdot q^2}{4\pi\epsilon_0 R_0} \left(1 - \frac{1}{n} \right)$

if N is the number of atomic ions rather than $2N$.

(b) If the linear chain is compressed so that $R_0 \rightarrow R_0 (1 - \delta)$ and δ is small, we can Taylor expand

$$f(x) = f(x_0) + \left. \frac{df}{dx} \right|_{x=x_0} (x - x_0) + \frac{1}{2} \left. \frac{d^2f}{dx^2} \right|_{x=x_0} (x - x_0)^2$$

with the mapping $x \rightarrow R_0 (1 - \delta)$, $x_0 \rightarrow R_0$, and $f \rightarrow U(r)$.

We get $U[R_0(1 - \delta)] - U(R_0) \equiv \Delta U = \frac{1}{2} \left. \frac{d^2U}{dR^2} \right|_{R=R_0} (R_0 \delta)^2$ with $\left. \frac{d^2U}{dR^2} \right|_{R=R_0} = \frac{2N \ln 2 q^2}{4\pi\epsilon_0 R_0^3} (n - 1)$

So the mechanical work per unit length is, $\Delta U' \equiv \Delta U / (2NR_0) = \frac{1}{2} C \delta^2 / R_0$ with $C = \frac{\ln 2 \cdot q^2}{4\pi\epsilon_0 R_0} (n - 1)$.

5.

(a) To get U_0 in terms of α , r , and R_0 , we use fact that in equilibrium

$$dU/dR|_{R_0} = 0 \Rightarrow \left. \frac{N}{2} \left[\frac{-z\lambda}{\rho} e^{-R/\rho} + \frac{\alpha q^2}{4\pi\epsilon_0 R^2} \right] \right|_{R=R_0} = 0 \text{ or } z\lambda e^{-R_0/\rho} = \frac{\alpha q^2 \rho}{4\pi\epsilon_0 R_0^2}$$

$$\text{So that, } U_0 = \frac{1}{2} N \left[\frac{\alpha q^2 \rho}{4\pi\epsilon_0 R_0^2} - \frac{\alpha q^2}{4\pi\epsilon_0 R_0} \right] = \frac{N\alpha q^2}{8\pi\epsilon_0 R_0} \left[\frac{\rho}{R_0} - 1 \right]$$

(b) For NaCl structure $R_0 =$ nearest neighbor distance $= a/2$.

$$\text{So } \rho = \left[\frac{4\pi\epsilon_0 a U_0}{N\alpha q^2} + 1 \right] \frac{a}{2} = (-0.87 + 1) \frac{a}{2} = 0.2726 \text{ Angstrom}$$

Where the last step uses $a = 4.215 \text{ Ang}$, $U_0/N = -5.20 \text{ eV/N}$, $\alpha = 1.7476$, and $q = e$

(c) We re-arrange the Madelung expression to get

$$\frac{2U}{N} + \frac{\alpha q^2}{4\pi\epsilon_0 R_0} = z\lambda \exp(-R_0/\rho) \text{ or } \lambda = \frac{\exp(a/2\rho)}{z} \left[\frac{2U}{N} + \frac{\alpha q^2}{2\pi\epsilon_0 a} \right]$$

which for $z = 6$ becomes $\lambda = (2279/6)[-10.4 + 11.94] \text{ eV}$

$$\text{or } \lambda = 584.9 \text{ eV} = 9.371 \times 10^{-17} \text{ J}$$

- (d) In zincblende structure, we expect ρ and λ to stay the same since they depend only on Mg and O pair. But α goes to 1.6381 because of the lattice change.

$$\text{So, given that } \rho = 0.2726 \text{ and } R_0 = 1.959 \text{ Ang}, \quad \frac{U_0}{N} = \frac{\alpha q^2}{8\pi\epsilon_0 R_0} \left[\frac{\rho}{R_0} - 1 \right] = -5.18 \text{ eV}$$

- 6 . (a) On cooling from $T = 753 \text{ K}$ to $T = 294 \text{ K}$: (solution courtesy of K. McGroddy).

$$\Delta a_{\text{GaN}} = 3.1945 - 3.1880 = 0.0065$$

$$\Delta a_{\text{sapphire}} = 4.7713 - 4.7577 = 0.0136$$

$$\epsilon = \Delta a/a = [0.0136 - 3^{1/2}(0.0065)]/(4.7577) = 5 \times 10^{-4} = \underline{0.05\%}$$

$$\underline{(b) \Delta U_{\text{elastic}} = \int \sigma d\epsilon = (0.5)Y\epsilon^2 = (0.5)(3.45 \times 10^{11} \text{ N/m}^2)(0.0005)^2 = \underline{4.3 \times 10^4 \text{ N/m}^2}}$$