**1.** For the HCP structure ABAB...the atoms in the B layer are equidistant from the atoms in the lower basal plane. The distance between an atom in the A layer and the atom in the B layer is equivalent to the distance between the atoms in the basal plane $a$. Also the height of the B layer is $c/2$. We can draw a right triangle with the hypothenuse being the distance between the atoms $a$ and two sides of length $c/2$ and $x$ as shown in Figure 1.
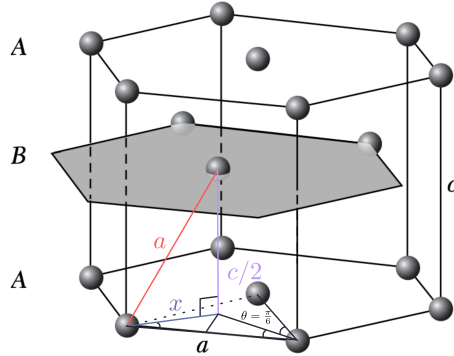


Figure 1: HCP structure (From Kittel)

To find $x$ we can project the B atom onto the basal plane and use trig to find that

$$x\cos\frac{\pi}{6} = \frac{a}{2} \rightarrow x = \frac{a}{\sqrt{3}}$$

So using the Pythagorean theorem we can find the distance between the atoms in the A and B layers

$$a^2 = \left(\frac{c}{2}\right)^2 + x^2$$

$$a^2 = \frac{c^2}{4} + \left(\frac{a}{\sqrt{3}}\right)^2$$

$$\frac{2}{3}a^2 = \frac{c^2}{4}$$

$$\frac{c}{a} = \sqrt{\frac{8}{3}} \approx 1.633$$

**2.** (a) Given

$$\mathbf{a}_1 = (\sqrt{3}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}}; \qquad \mathbf{a}_2 = -(\sqrt{3}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}}; \qquad \mathbf{a}_3 = c\hat{\mathbf{z}}$$

the volume of the primitive cell is equivalent to the volume of the parallelepiped:

$$V_c = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$$

$$= \mathbf{a}_1 \cdot \det \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ -\sqrt{3}a/2 & a/2 & 0 \\ 0 & 0 & c \end{vmatrix}$$

$$= \left(\frac{\sqrt{3}a}{2}\hat{\mathbf{x}} + \frac{a}{2}\hat{\mathbf{y}}\right) \cdot \left(\frac{ac}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}ac}{2}\hat{\mathbf{y}}\right)$$

$$= \frac{\sqrt{3}a^2c}{4} + \frac{\sqrt{3}a^2c}{4}$$

$$= \frac{\sqrt{3}a^2c}{2}$$

(b) The first reciprocal lattice vector is

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_c}$$

$$= 2\pi \frac{\left(\frac{ac}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}ac}{2}\hat{\mathbf{y}}\right)}{\frac{\sqrt{3}a^2c}{2}}$$

$$= 2\pi \frac{\hat{\mathbf{x}} + \sqrt{3}\hat{\mathbf{y}}}{\sqrt{3}a}$$

$$= \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{\mathbf{x}} + \hat{\mathbf{y}}\right)$$

The other reciprocal lattice vectors can be found similarly:

$$\mathbf{a}_3 \times \mathbf{a}_1 = \det \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ 0 & 0 & c \\ \sqrt{3}a/2 & a/2 & 0 \end{vmatrix} = -\frac{ac}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}ac}{2}\hat{\mathbf{y}}$$

so

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V_c} = \frac{2\pi}{a}\left(-\frac{1}{\sqrt{3}}\hat{\mathbf{x}} + \hat{\mathbf{y}}\right)$$

and

$$\mathbf{a}_1 \times \mathbf{a}_2 = \det \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ \sqrt{3}a/2 & a/2 & 0 \\ -\sqrt{3}a/2 & a/2 & 0 \end{vmatrix} = (\sqrt{3}a^2/4 + \sqrt{3}a^2/4)\hat{\mathbf{z}} = \frac{\sqrt{3}a^2}{2}\hat{\mathbf{z}}$$

so

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V_c} = \frac{2\pi}{c}\hat{\mathbf{z}}$$

(c) A sketch of the 2D Brillouin zone is a hexagon as shown in Figure 2.
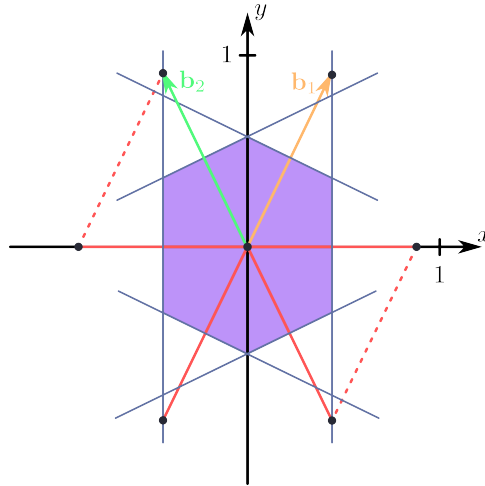


Figure 2: 2D Brillouin zone on $xy$ plane

**3.** (a) The total potential energy is

$$U(R) = N\left(\frac{A}{R^n} - \frac{\alpha q^2}{R}\right)$$

where the Madelung constant for a 1D chain of ions is $\alpha = 2\ln 2$, and we replace the usual repulsive potential $\lambda \exp(-R/p)$ with $A/R^n$. Taking the derivative with respect to $R$ an finding the equilibrium seperation at a critical point:

$$\frac{\mathrm{d}U}{\mathrm{d}R} = N\left(-\frac{nA}{R^{n+1}} + \frac{\alpha q^2}{R^2}\right) = 0$$

$$\frac{NA}{R^{N+1}} = \frac{\alpha q^2}{R^2}$$

$$\frac{R^{n+1}}{R^2} = \frac{nA}{\alpha q^2}$$

$$R_o^{n-1} = \frac{nA}{\alpha q^2}$$

$$A = \frac{\alpha q^2 R_o^{n-1}}{n}$$

substituting back into the potential energy:

$$U(R_o) = N\left(\frac{\alpha q^2 R_o^{n-1}}{n R_o^n} - \frac{\alpha q^2}{R_o}\right)$$

$$= N\left(\frac{\alpha q^2}{n R_o} - \frac{\alpha q^2}{R_o}\right)$$

$$= \frac{N\alpha q^2}{R_o}\left(\frac{1}{n} - 1\right)$$

$$U(R_o) = -\frac{2Nq^2 \ln 2}{R_o}\left(1 - \frac{1}{n}\right)$$

(b) Approximating the potential around $x$ using Taylor expansion $f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2$:

$$U(R_o(1-\delta)) = U(R_o + (-R_o\delta))$$

$$= U(R_o) - [U'(R_o)](R_o\delta) + \frac{1}{2}[U''(R_o)](R_o\delta)^2 + \dots$$

and since $\frac{\mathrm{d}U}{\mathrm{d}R} = 0$ at $R_o$, the second term is zero. And the second order derivative gives

$$\frac{\mathrm{d}^2 U}{\mathrm{d}R^2} = N\left(\frac{n(n+1)A}{R^{n+2}} - \frac{2\alpha q^2}{R^3}\right)\bigg|_{R=R_o}$$

$$\text{using} \quad R_o^{n-1} = \frac{nA}{\alpha q^2}$$

$$= N\left(\frac{n(n+1)A}{\frac{nA}{\alpha q^2}R_o^3} - \frac{2\alpha q^2}{R_o^3}\right)$$

$$= N\left(\frac{(n+1)\alpha q^2}{R_o^3} - \frac{2\alpha q^2}{R_o^3}\right)$$

$$= \frac{N\alpha q^2}{R_o^3}((n+1) - 2)$$

$$\frac{\mathrm{d}^2 U}{\mathrm{d}R^2} = \frac{N\alpha q^2}{R_o^3}(n-1)$$

so potential is approximately

$$U(R_o(1-\delta)) \approx U(R_o) + \frac{1}{2}\frac{N\alpha q^2}{R_o^3}(n-1)(R_o\delta)^2$$

so the leading coefficient is (ignoring the $\frac{1}{2}\delta^2$ part)

$$C = \frac{N\alpha q^2}{R_o^3}(n-1)R_o^2$$

To cancel the $N$ we can use that fact that compressing to the unit length makes the seperation between ions $2NR_o = 1$, so $N = 1/(2R_o)$, so

$$C = \frac{1}{2R_o}\frac{\alpha q^2}{R_o^3}(n-1)R_o^2 = \frac{\alpha q^2}{2R_o^2}(n-1)$$

and using the Madelung constant $\alpha = 2\ln 2$, the leading term is finally

$$C = \frac{(n-1)q^2\ln 2}{R_o^2}$$

so the work done is

$$W = \Delta U = U((R_o\delta)) - U(R_o)$$
$$\approx U(R_o) + \frac{1}{2}C\delta^2 - U(R_o)$$
$$W \approx \frac{1}{2}C^2\delta^2$$

where the leading term is indead in the order of $\frac{1}{2}C\delta^2$.