

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 hypotenuse being the distance between the atoms  $a$  and two sides of length  $c/2$  and  $x$  as shown in Figure 1.

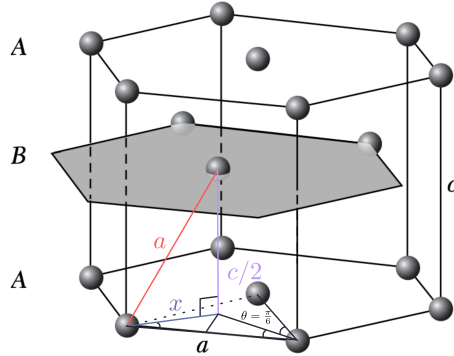


Figure 1: HCP structure (From Kittel)

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

$$\begin{aligned} a^2 &= \left(\frac{c}{2}\right)^2 + x^2 \\ a^2 &= \frac{c^2}{4} + \left(\frac{a}{\sqrt{3}}\right)^2 \\ \frac{2}{3}a^2 &= \frac{c^2}{4} \\ \frac{c}{a} &= \sqrt{\frac{8}{3}} \approx 1.633 \end{aligned}$$

2. (a) Given

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

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

$$\begin{aligned} V_c &= \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) \\ &= \mathbf{a}_1 \cdot \det \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ -\sqrt{3}a/2 & a/2 & 0 \\ 0 & 0 & c \end{vmatrix} \\ &= \left(\frac{\sqrt{3}a}{2}\hat{\mathbf{x}} + \frac{a}{2}\hat{\mathbf{y}}\right) \cdot \left(\frac{ac}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}ac}{2}\hat{\mathbf{y}}\right) \\ &= \frac{\sqrt{3}a^2c}{4} + \frac{\sqrt{3}a^2c}{4} \\ &= \frac{\sqrt{3}a^2c}{2} \end{aligned}$$

(b) The first reciprocal lattice vector is

$$\begin{aligned}
 \mathbf{b}_1 &= 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_c} \\
 &= 2\pi \frac{\left(\frac{ac}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}ac}{2}\hat{\mathbf{y}}\right)}{\frac{\sqrt{3}a^2c}{2}} \\
 &= 2\pi \frac{\hat{\mathbf{x}} + \sqrt{3}\hat{\mathbf{y}}}{\sqrt{3}a} \\
 &= \frac{2\pi}{a} \left(\frac{1}{\sqrt{3}}\hat{\mathbf{x}} + \hat{\mathbf{y}}\right)
 \end{aligned}$$

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.

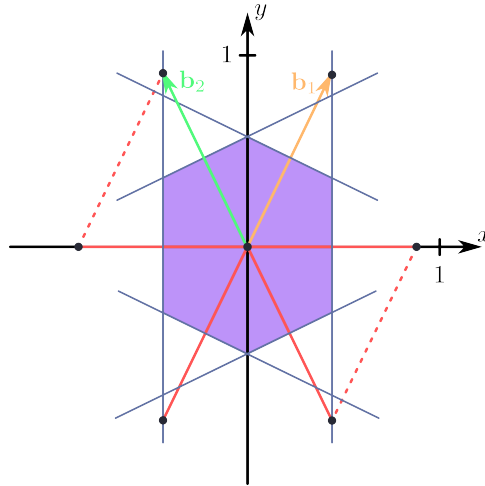


Figure 2: 2D Brillouin zone on  $xy$  plane

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  $R$  and finding the equilibrium separation at a critical point:

$$\begin{aligned}\frac{dU}{dR} &= N \left( -\frac{nA}{R^{n+1}} + \frac{\alpha q^2}{R^2} \right) = 0 \\ \frac{NA}{R^{n+1}} &= \frac{\alpha q^2}{R^2} \\ \frac{R^{n+1}}{R^2} &= \frac{nA}{\alpha q^2} \\ R_o^{n-1} &= \frac{nA}{\alpha q^2} \\ A &= \frac{\alpha q^2 R_o^{n-1}}{n}\end{aligned}$$

substituting back into the potential energy:

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

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

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

and since  $\frac{dU}{dR} = 0$  at  $R_o$ , the second term is zero. And the second order derivative gives

$$\begin{aligned}\frac{d^2U}{dR^2} &= N \left( \frac{n(n+1)A}{R^{n+2}} - \frac{2\alpha q^2}{R^3} \right) \Big|_{R=R_o} \\ \text{using } R_o^{n-1} &= \frac{nA}{\alpha q^2} \\ &= N \left( \frac{n(n+1)A}{\frac{nA}{\alpha q^2} R_o^3} - \frac{2\alpha q^2}{R_o^3} \right) \\ &= N \left( \frac{(n+1)\alpha q^2}{R_o^3} - \frac{2\alpha q^2}{R_o^3} \right) \\ &= \frac{N \alpha q^2}{R_o^3} ((n+1) - 2) \\ \frac{d^2U}{dR^2} &= \frac{N \alpha q^2}{R_o^3} (n-1)\end{aligned}$$

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 separation 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

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

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