PYQ Solution [GATE]

(Chapter 3 Crystal Binding)

Ans. 1: 1.74

Solution: $U(r) = -\frac{Ae^2}{4\pi\varepsilon_0 r} + \frac{K}{r^n}$, where A is Modelung Constant,

Given: $n = 9$, binding energy per molecule $(U_0) = 7.95\ eV$ and lattice parameter $a = 0.563\ nm$.

The potential energy will be minimum at the equilibrium spacing r_0, so

$$\left[\frac{dU}{dr}\right]_{r=r_0} = \frac{Ae^2}{4\pi\varepsilon_0 r_0^2} - \frac{nK}{r_0^{n+1}} = 0$$

$$\frac{Ae^2}{4\pi\varepsilon_0 r_0^2} = \frac{nK}{r_0^{n+1}} \qquad \Rightarrow K = \frac{Ae^2 r_0^{n-1}}{4\pi\varepsilon_0 n}$$

Thus, Binding energy of molecule or lattice energy will be

$$U_0 = [U]_{r=r_0} = -\frac{Ae^2}{4\pi\varepsilon_0 r_0} + \frac{Ae^2 r_0^{n-1}}{4\pi\varepsilon_0 n r_0^n} = -\left[\frac{Ae^2}{4\pi\varepsilon_0 r_0}\right]\left[1 - \frac{1}{n}\right]$$

Modelung constant $(A) = U_0 \times \frac{4\pi\varepsilon_0 r_0}{e^2} \times \frac{n}{n-1}$ and the inter atomic separation is $r_0 = \frac{a}{2} = 0.28\ nm$.

$$\Rightarrow A = \frac{7.95\times 1.6\times 10^{-19} J \times \left(0.28\times 10^{-9}\right)\times 9}{9\times 10^9 \times \left(1.6\times 10^{-19} J\right)^2 \times 8} = 0.1739\times 10 = 1.74$$

$$\Rightarrow A = 1.74$$

Ans. 2: 1

Solution: Given that $E(R) = \frac{0.5}{R^{12}} - \frac{1}{R^6}$

For equilibrium separation, $\frac{dE}{dR} = 0$

$$\Rightarrow \frac{dE}{dR} = -\frac{12\times 0.5}{R^{13}} + \frac{6}{R^7} = 0 \Rightarrow \frac{1}{R^7}\left[\frac{-6}{R^6} + 6\right] = 0 \Rightarrow R^6 = 1 \Rightarrow R = 1$$

Ans. 3: (a)

Solution: At $r = r_0$, $\left.\frac{dE}{dr}\right|_{r=r_0} = 0 \Rightarrow \frac{\alpha e^2}{4\pi\varepsilon_0 r_0^2} - \frac{9B}{r_0^{10}} = 0 \Rightarrow B = \frac{\alpha e^2 r_0^8}{36\pi\varepsilon_0}$

Ans. 4: 1.09

Solution: $U(R)=2N\in\left[p\left(\frac{\sigma}{R}\right)^{12}-q\left(\frac{\sigma}{R}\right)^{6}\right],\ p=12.13\ \&\ q=14.45$

$$\frac{dU}{dR}=0 \quad \Rightarrow 2N\in\left[\frac{-12p}{R}\left(\frac{\sigma}{R}\right)^{12}+\frac{6q}{R}\left(\frac{\sigma}{R}\right)^{6}\right]=0 \quad \Rightarrow 2p\left(\frac{\sigma}{R}\right)^{6}=q \quad \Rightarrow R=\left(\frac{2p}{q}\right)^{1/6}\sigma$$

Now put the values of p and q in above equation :

$$R=\left(\frac{2\times 12.13}{14.45}\right)^{1/6}\sigma=(1.679)^{1/6}\sigma=1.09\sigma$$

Thus $R=1.09\sigma$

PYQ Solution [NET]

Ans. 1: (d)

Solution: Given $V(r) = -\frac{a}{r^6} + \frac{b}{r^{12}}$. At equilibrium separation, $\left.\frac{dV(r)}{dr}\right|_{r=r_0} = 0$

$$\frac{dV(r)}{dr} = \frac{6a}{r_0^7} - \frac{12b}{r_0^{13}} = 0 \Rightarrow \frac{6a}{r_0^7} = \frac{12b}{r_0^{13}} \Rightarrow r_0^6 = \frac{2b}{a}$$

The value of potential at equilibrium will be

$$V(r_0) = -\frac{a}{r_0^6} + \frac{b}{r_0^{12}} = \frac{1}{r_0^6}\left[-a + \frac{b}{r_0^6}\right] = -\frac{a^2}{2b} + \frac{a^2}{4b} = \frac{-a^2}{4b}.$$