[Solution] *Theoretical Question 3*

Thermal Vibration of Surface Atoms

(1) (a) The wavelength of the incident electron is

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}}$$
$$= \frac{6.63\times10^{-34}}{\sqrt{2\times9.11\times10^{-31}\times1.60\times10^{-19}\times64.0}}$$
$$= 1.53\times10^{-10}\,m = 1.53\,\mathring{A}$$

(b) Consider the interference between the atomic rows on the surface as shown in Fig. 3c.

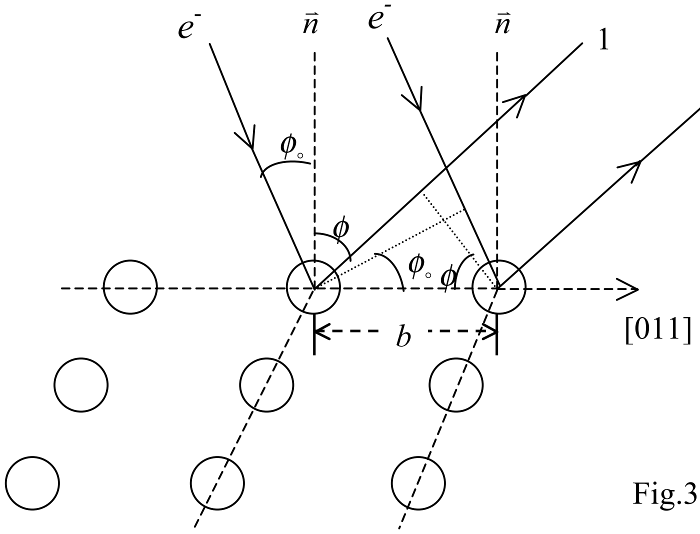

Fig.3c

The path difference between electron beam 1 and 2 is

$$\Delta\ell = b(\sin\phi - \sin\phi_\circ) = n\lambda$$

Given $\phi_\circ = 15.0^\circ$, $\lambda = 1.53\,\mathring{A}$ and $b = \frac{a}{\sqrt{2}} = \frac{3.92}{\sqrt{2}} = 2.77\,\mathring{A}$, two solutions are possible.

(i) When $n = 0$, $\phi = \phi_\circ = 15.0^\circ$ (Answer 1)

(ii) When $n = 1$

$$\Delta\ell = 2.77(\sin\phi - \sin 15^\circ) = 1\times1.53$$

$$\sin\phi = \frac{1.53 + 0.72}{2.77} = 0.812$$

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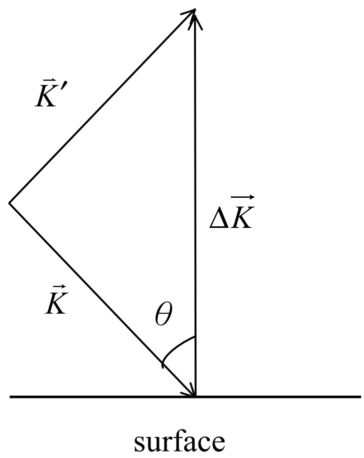
$$\phi = 54.3^\circ \qquad \text{(Answer 2)}$$

For $n = 2$, no solution exists as $\Delta\ell = 2.77(\sin\phi - \sin 15^\circ) = 2\times 1.53$ and $\sin\phi > 1$.

(2) $I = I_0 \exp\langle -(\vec{u}\cdot\Delta\vec{K})^2\rangle$

Fig. 3d



For the specularly reflected beam, we have from Fig. 3d

$$\Delta\vec{K} = \vec{K}' - \vec{K} = 2K\cos\theta \quad \hat{x}$$

where $\hat{x}$ is the unit vector in the direction of the surface normal. Take the x-component of $\vec{u}$, we then obtain

$$I = I_0 e^{-<u_x^2(t)\cdot 4K^2\cos^2\theta>} = I_0 e^{-4K^2\cos^2\theta <u_x{}^2(t)>} \qquad (2)$$

The vibration in the direction of the surface normal of the surface atoms is simple harmonic, take

$$u_x(t) = A\cos\omega t$$

$$\because \qquad \langle u_x{}^2(t)\rangle = \frac{1}{\tau}\int_0^\tau u^2 dt = \frac{1}{\tau}\int_0^\tau A^2\cos^2\omega t\, dt = \frac{A^2}{\tau}\cdot\frac{\tau}{2} = \frac{A^2}{2}$$

$$\therefore \quad A^2 = 2\langle u_x{}^2(t)\rangle$$

The total energy E is thus given by

$$E = \frac{1}{2}CA^2 = \frac{1}{2}C\cdot 2 < u_x{}^2(t) > \; = \; C < u_x{}^2(t) > \; = \; m'\omega^2 < u_x{}^2(t) >$$

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Therefore, one obtains

$$< u_x^2(t) > \; = \; E / (m'\omega^2)$$

$$E = m'\omega^2 < u_x^2 > = k_B T$$

where m' is the mass of the atom. From either of the above two equations, one then has the following equality

$$< u_x^2 > = \frac{k_B T}{m'\omega^2} = \frac{k_B T}{m' 4\pi^2 f^2} \qquad (3)$$

From eq. (3) and eq. (2), one obtains

$$I = I_0 e^{-4K^2 \cos^2\theta \frac{k_B T}{m' 4\pi^2 f^2}}$$

where $K = \frac{2\pi p}{h} = \frac{2\pi}{\lambda}$. Accordingly,

$$I = I_0 e^{-\frac{4k_B \cos^2\theta}{m' f^2 \lambda^2} T} = I_0 e^{-M'T} \qquad (4)$$

and

$$\ell n \frac{I}{I_0} = -M'T$$

From the plot of $\ell n \frac{I}{I_0}$ versus T, one obtains the slope

$$M' = \frac{4k_B \cos^2\theta}{m' f^2 \lambda^2} \qquad (5)$$

The slope of the curve can be estimated from Fig. 3b and leads to the result

$$M' = 2.3\times10^{-3}.$$

Using the following data in Eq.(5),

$$k_B = 1.38\times10^{-23} J/K$$

$$\lambda = 1.53\times10^{-10} m$$

$$m' = 195.1\times10^{-3}/(6.02\times10^{23}) = 3.24 \times10^{-25} \; kg/atom$$

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one finds

$$2.3\times10^{-3} = \frac{4\times1.38\times10^{-23}\cdot cos^2 15^\circ}{\frac{195.1\times10^{-3}}{6.02\times10^{23}}\times f^2\times(1.53\times10^{-10})^2}$$

The solution for frequency is then

$$f^2 = 3.0\times10^{24}\,\text{(new)} \Rightarrow \quad f = 1.7\times10^{12}\,Hz \quad \text{Answer (a)}$$

From $< u_x{}^2 >= \dfrac{k_B T}{m' 4\pi^2 f^2}$, $T = 300K$, one finally obtains

$$< u_x{}^2 >= \frac{1.38\times10^{-23}\cdot300}{\frac{195.1\times10^{-3}}{6.02\times10^{23}}\times4\pi^2\times3.0\times10^{24}} = 1.1\times10^{-22}\,m^2\,\text{(new)}$$

and

$$\sqrt{< u_x{}^2 >} = 1.0\times10^{-11}\,m = 0.10\,\mathring{A}\,\text{(new)}$$

Ans