STATE UNIVERSITY OF NEW YORK AT BUFFALO

Department of Mechanical and Aerospace Engineering

MEA 589 Diffraction, Microscopy and Spectroscopy Techniques

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January 29, 2004

HOMEWORK NO. 2

S O L U T I O N

Problem 1 (14%)

(a) Amplitude = 2

(b) The Wave number $k = \frac{2\pi}{\lambda} = \frac{2\pi}{30}\ \text{cm}^{-1}$

Thus, the wavelength $\lambda = \underline{\underline{30\ \text{cm}}}$

(c) Using Eq. (2.3) in the notes, the angular frequency

$$\omega = 2\pi\ \nu = \frac{2\pi}{0.01}\ \text{sec}^{-1}$$

Thus, the frequency

$$\nu = \frac{1}{0.01}\ \text{sec}^{-1} = \underline{\underline{100\ \text{sec}^{-1}}}$$

(d) The speed of propagation or the phase velocity is given by Eq. (2.4) in the notes.

$$v_p = \nu\lambda = (100\ \text{sec}^{-1})(30\ \text{cm})$$

$$= \underline{\underline{3000\ \text{cm} \cdot \text{sec}^{-1}}}$$

Problem 2 (14%)

Using Eq. (2.19) in the notes,

$$\lambda = \sqrt{\frac{h^2}{2mE}}$$

$$h = 6.6252 \times 10^{-27}\ \text{erg. sec}$$

$$= 6.6252 \times 10^{-34}\ \text{joule. sec}$$

$$m = 9.1 \times 10^{-31}\ \text{kg}$$

$$E = 100\ \text{eV} = (100\text{eV})(1.6 \times 10^{-10}\ \text{joule/eV})$$

$$= 1.6 \times 10^{-17}\ \text{joule}$$

Hence,

$$\lambda = \sqrt{\frac{(6.6252 \times 10^{-34})^2\ \text{joule}^2\ \text{sec}^2}{2(9.1 \times 10^{-31}\text{kg})(1.6 \times 10^{-17}\ \text{joule})}}$$

$$= 1.2 \times 10^{-10}\text{m}$$

$$= \underline{\underline{1.2\ \text{Å}}}$$

This is the same order of magnitude as the size of an atom or the spacing between adjacent planes of atoms in a solid. As will be seen in Chapter 3, this characteristic makes an electron beam suitable for diffraction in solids.

Problem 3 (16%)

$$\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = \begin{vmatrix} 1 & 2 & -1 \\ 0 & 1 & 1 \\ 1 & -1 & 0 \end{vmatrix}$$

$$= 1(0+1) - 2(0-1) - 1(0-1)$$

$$= \underline{\underline{4}}$$

Problem 4 (16%)

According to Eq. (2.33) in the notes,

$$\vec{b}_1 = \frac{2\pi}{\Omega_a}(\vec{a}_2 \times \vec{a}_3) \ ,$$

where Ω_a is the volume of the unit cell in real space.

The volume Ω_b of the unit cell in reciprocal space is given by

$$\Omega_b = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$$

$$= \left(\frac{2\pi}{\Omega_a}\right)[(\vec{a}_2 \times \vec{a}_3) \cdot (\vec{b}_2 \times \vec{b}_3)]$$

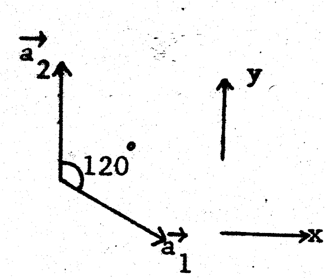
$$= \left(\frac{2\pi}{\Omega_a}\right) [(\vec{a}_2 \cdot \vec{b}_2)(\vec{a}_3 \cdot \vec{b}_3) - (\vec{a}_2 \cdot \vec{b}_3)(\vec{a}_3 \cdot \vec{b}_2)]$$

$$= \left(\frac{2\pi}{\Omega_a}\right)[(2\pi)^2 - 0]$$

$$= \underline{\underline{\frac{(2\pi)^3}{\Omega_a}}}$$

Problem 5 (40%)

(a)



(b) $|\vec{a}_1| = a\sqrt{(\frac{\sqrt{3}}{2})^2 + (-\frac{1}{2})^2} = a$

$|\vec{a}_2| = a\sqrt{0^2 + 1^2} = a$

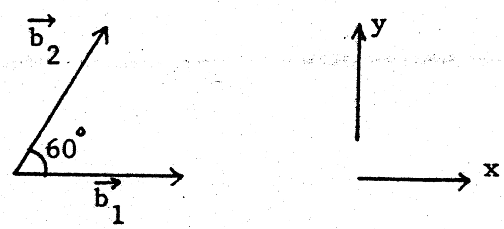
(c) $\Omega_a = \vec{a}_1 \times \vec{a}_2 = a^2 \frac{\sqrt{3}}{2}$

(d) By inspection, knowing that $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$, we obtain

$$\vec{b}_1 = \frac{2\pi}{a}\left(\frac{2}{\sqrt{3}}, 0\right)$$

$$\vec{b}_2 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, 1\right)$$

(e)



(f) $|\vec{b}_1| = \frac{2\pi}{a}\frac{2}{\sqrt{3}}$

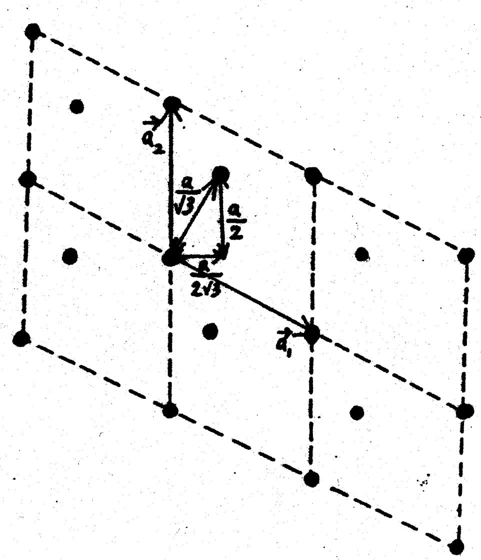
$|\vec{b}_2| = \frac{2\pi}{a}\sqrt{\left(\frac{1}{\sqrt{3}}\right)^2 + 1^2} = \frac{2\pi}{a}\frac{2}{\sqrt{3}}$

(g) $\Omega_b = \vec{b}_1 \times \vec{b}_2 = \frac{4\pi^2}{a^2}\frac{2}{\sqrt{3}} = \frac{8\pi^2}{\sqrt{3}a^2}$.

Note that $\Omega_b = \frac{(2\pi)^2}{\Omega_a}$,

which is the two-dimensional version of Eq. (2.34) in the notes.

(h)



Problem 6

Naturally occurring copper has an atomic weight of 63.55. Its principal isotopes are Cu^{63} and Cu^{65}. What is the abundance (in atomic percent) of each isotope?

$$x\ Cu^{63} + y\ Cu^{65} = Cu^{63.55}$$

or

$$63x + 65y = 63.55$$

or

$$63x + 65(1-x) = 63.55$$

or

$$65 - 2x = 63.55$$

or

$$2x = 65.00 - 63.55$$

or

$$x = 0.725$$

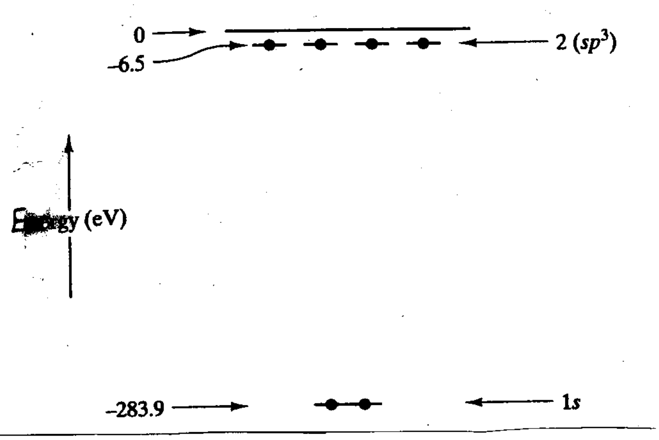
and

$$y = 1 - x = 0.275$$

giving:

$$\underline{\underline{72.5\%\ Cu^{63} \text{ and } 27.5\%\ Cu^{65}}}$$

Problem 7



The orbital electrons of an atom can be ejected by exposure to a beam of electromagnetic radiation. Specifically, an electron can be ejected by a photon with energy greater than or equal to the electron's binding energy. Given that the photon energy (E) is equal to hc/λ, where h is Planck's constant, c the speed of light, and λ the wavelength, calculate the minimum wavelength of radiation necessary to eject a 1s electron from a ^{12}C atom. (See Figure 2-3.)

From Figure 2–3, $|E| = 283.9\,eV$.

Then, $\lambda_{min} = \frac{hc}{E}$

$$= \frac{(0.6626\times10^{-33}\,J\cdot s)(0.2998\times10^{9}\,m/s)}{(283.9\,eV)(1\,J/6.242\times10^{18}\,eV)}$$

$$= 4.37\times10^{-9}\,m \times 1\,nm/10^{-9}\,m$$

$$= \underline{\underline{4.37\,nm}}$$

Note: We use the magnitude of the electron binding energy rather than the arbitrary negative sign convention to provide a physically meaningful positive wavelength.

Problem 8

Once the 1s electron is ejected from a ^{12}C atom, as described in Problem 2.10, there is a tendency for one of the 2(sp^3) electrons to drop into the 1s level. The result is the emission of a photon with an energy precisely equal to the energy change associated with the electron transition. Calculate the wavelength of the photon that would be emitted from a ^{12}C atom. (You will note various examples of this concept throughout the text in relation to the chemical analysis of engineering materials.)

From Figure 2-3 and again using the magnitude of the energies involved,

$$|\Delta E| = |-283.9 - (-6.5)|\,eV$$

$$= 277.4\ eV$$

or

$$\lambda = \frac{hc}{\Delta E}$$

$$= \frac{(0.6626\times10^{-33}\,J\cdot s)(0.2998\times10^{9}\,m/s)}{(277.4\,eV)(1J/6.242\times10^{18}\,eV)}$$

$$= 4.47\times10^{-9}\,m \times 1\,nm/10^{-9}\,m$$

$$= \underline{\underline{4.47\,nm}}$$

Problem 9

The mechanism for producing a photon of specific energy is outlined in Problem 2.11. The magnitude of photon energy increases with the atomic number of the atom from which emission occurs. (This is due to the stronger binding forces between the negative electrons and the positive nucleus as the numbers of protons and electrons increase with atomic number.) As noted in Problem 2.10, $E = hc/\lambda$, which means that a higher-energy photon will have a shorter wavelength. Verify that higher atomic number materials will emit higher-energy, shorter-wavelength photons by calculating E and λ for emission from iron (atomic number 26 compared to 6 for carbon), given that the energy levels for the first two electron orbitals in iron are at $-7{,}112$eV and -708eV.

$$|\Delta E| = |-7{,}112 - (-708)|\,eV = 6404\,eV$$

or $$\lambda = \frac{hc}{\Delta E} = \frac{(0.6626\times10^{-33}\,J\cdot s)(0.2998\times10^{9}\,m/s)}{(6404\,eV)(1J/6.242\times10^{18}\,eV)}$$

$$= 1.94\times10^{-10}\,m \times 1\,nm/10^{-9}\,m = \underline{\underline{0.194\,nm}}$$