STATE UNIVERSITY OF NEW YORK AT BUFFALO

Department of Mechanical and Aerospace Engineering

MEA 589 Diffraction, Microscopy and Spectroscopy Techniques

Prof. D.D.L. Chung

January 22, 2004

HOMEWORK NO. 2

Problem 1 (14%)

The equation of a certain traveling transverse wave is

$$y = 2 \sin 2\pi \left(\frac{t}{0.01} - \frac{x}{30}\right),$$

where x and y are in centimeters and t is in seconds. What are (a) the amplitude, (b) the wavelength, (c) the frequency, and (d) the speed of propagation of the wave?

Problem 2 (14%)

What wavelength is associated with a beam of electrons whose kinetic energy is 100 eV? The mass of an electron is

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

$$1\text{eV} = 1.6 \times 10^{-19} \text{ joule}$$

Problem 3 (16%)

A parallelepiped is defined by the vectors $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$, where

$$\vec{a}_1 = (1, 2, -1)$$

$$\vec{a}_2 = (0, 1, 1)$$

$$\vec{a}_3 = (1, -1, 0)$$

Calculate the volume of the parallelepiped by using the triple scalar product

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \begin{vmatrix} a_{1x} & a_{1y} & a_{1z} \\ a_{2x} & a_{2y} & a_{2z} \\ a_{3x} & a_{3y} & a_{3z} \end{vmatrix}$$

$$= a_{1x}(a_{2y}\, a_{3z} - a_{2z}\, a_{3y})$$

$$- a_{1y}(a_{2x}\, a_{3z} - a_{2z}\, a_{3x})$$

$$+ a_{1z}(a_{2x}\, a_{3y} - a_{2y}\, a_{3x})$$

Problem 4 (16%)

Prove that the volume of a unit cell in reciprocal space ~~equals~~ is related to the inverse of the volume of the associated unit cell in real space.

HINT: $(\vec{A} \times \vec{B}) \cdot (\vec{C} \times \vec{D}) = (\vec{A} \cdot \vec{C})(\vec{B} \cdot \vec{D}) - (\vec{A} \cdot \vec{D})(\vec{B} \cdot \vec{C})$, where $\vec{A}$, $\vec{B}$, $\vec{C}$, and $\vec{D}$ are vectors.

Problem 5 (40%)

A two-dimensional lattice is defined by the fundamental translation vectors

$$\vec{a}_1 = a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$$

$$\vec{a}_2 = a(0,1)$$

(4%)(a) Sketch the vectors $\vec{a}_1$ and $\vec{a}_2$. Indicate the x and y directions on the sketch.

(4%)(b) Give the magnitudes of $\vec{a}_1$ and $\vec{a}_2$.

(4%)(c) Calculate the area of the unit cell in real space by using the cross product

$$\Omega_a = \vec{a}_1 \times \vec{a}_2 = \begin{vmatrix} a_{1x} & a_{1y} \\ a_{2x} & a_{2y} \end{vmatrix} = a_{1x}\, a_{2y} - a_{1y}\, a_{2x}$$

(8%)(d) Obtain the fundamental translation vectors $\vec{b}_1$ and $\vec{b}_2$ for the reciprocal lattice.

(4%)(e) Sketch the vectors $\vec{b}_1$ and $\vec{b}_2$. Indicate the x and y directions on the sketch.

(4%)(f) Give the magnitudes of $\vec{b}_1$ and $\vec{b}_2$.

(4%)(g) Calculate the area of the unit cell in reciprocal space.

(8%)(h) Consider a basis containing two atoms. The lattice point at (0,0) is associated with two atoms at (0,0) and $\left(\frac{a}{2\sqrt{3}}, \frac{a}{2}\right)$. By repeating this basis at every lattice point, a two-dimensional crystal structure is generated. Sketch this crystal structure, indicating each atom by a solid circle of arbitrary size. Indicate $\vec{a}_1$ and $\vec{a}_2$ in the sketch.

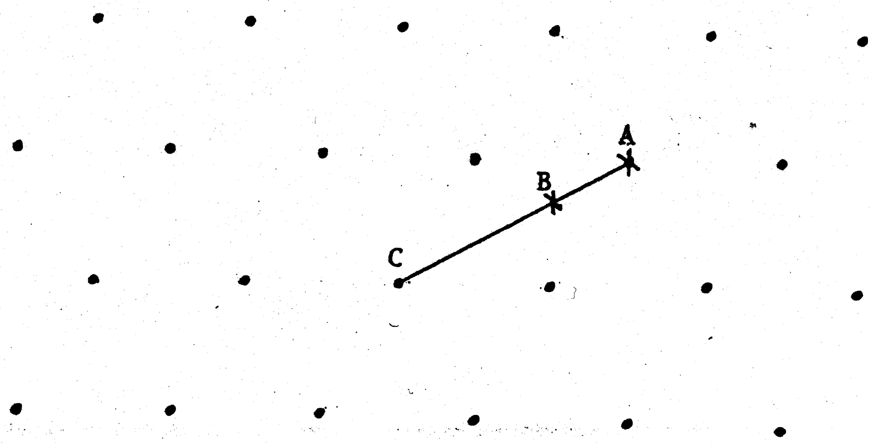

Fig. 3 A basis for the lattice of Fig. 2.

(6%) (e) What is the coordination number of the two-dimensional crystal structure obtained in (d)?

(6%) (f) The lattice constant is a, as indicated in Fig. 2. Assume that nearest neighbor atoms touch each other in this crystal structure, give the relationship between a and the atomic radius r.

Problem 3

Lead is FCC with atomic radius 1.750 Å. What is the volume of its unit cell?

Problem 4

Magnesium is HCP and has nearly spherical atoms with a radius of ~1.61 Å. What is its density? For Mg, $\frac{c}{a} = 1.62$. Hint: $a = 2r$ for HCP.

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?

Problem 7

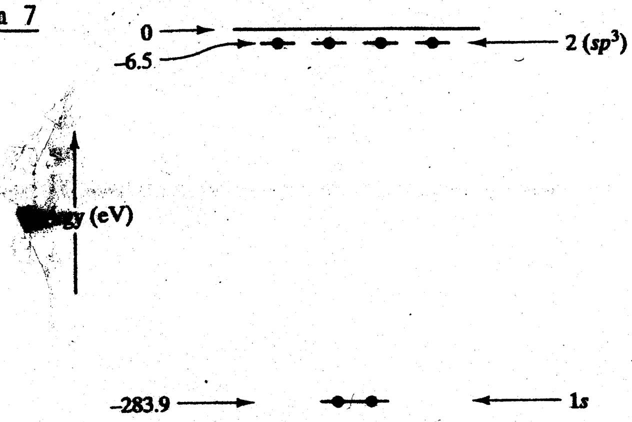

Figure 2-3 *Energy-level diagram for the orbital electrons in a ^{12}C atom. Notice the sign convention. An attractive energy is negative. The 1s electrons are closer to the nucleus (see Figure 2–1) and more strongly bound (binding energy = −283.9 eV). The outer orbital electrons have a binding energy of only −6.5 eV. The zero level of binding energy corresponds to an electron completely removed from the attractive potential of the nucleus.*

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 maximum wavelength of radiation (corresponding to the minimum energy) necessary to eject a 1s electron from a C^{12} atom. (See Figure 2–3.)

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.)

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 −7,112eV and −708eV.