Name________________________________ ID#_______________________________

MSE 333

Principles of Materials Characterization and Analysis

Prof. Kannan M. Krishnan

Mid-Term

60 Minutes + 20 mins (for online submission issues)

This is a **closed book** exam

If something is not clear, make your best assumption and state it.

The time for each problem is proportional to its points. Use it wisely.

Honor Code

I have not provided or taken help from anyone or any others sources (books, course pack, web sites, class or other written notes etc.)

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Signature Date

Some formulas you may need --

$$\mathbf{a^*} = 2\pi(\mathbf{b \times c}) / \mathbf{a}.(\mathbf{b \times c})$$

$$\mathbf{b^*} = 2\pi(\mathbf{c \times a}) / \mathbf{b}.(\mathbf{c \times a})$$

$$\mathbf{c^*} = 2\pi(\mathbf{a \times b}) / \mathbf{c}.(\mathbf{a \times b})$$

$$E_{\mathrm{kin}} = hf - |E_{\mathrm{B}}|$$

$$E_{\mathrm{kin}} = hf - |E_{\mathrm{B}}| - \Phi$$

$$E_n = -\frac{m_e Z^2 e^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} = -13.606\frac{Z^2}{n^2}\ (\mathrm{eV})$$

$$\lambda = \frac{h}{p}$$

$$I_x = I_0 \exp(-\mu x)$$

$$N(E) = 4\pi\left(\frac{2m_e}{h^2}\right)^{3/2} E^{1/2}$$

$$E_{vib} = \frac{1}{2}A(R-R_0)^2$$

$$E_{vib,n} = (n+1/2)hf_{vib}$$

$$\mu_{Ind} = \alpha_0 E_0 \cos(2\pi f_I t) + \frac{\alpha_1 E_0}{2}\left[\cos 2\pi(f_I - f_{\mathrm{int}})t + \cos 2\pi(f_I + f_{\mathrm{int}})t\right]$$

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

$$n\lambda = 2d\sin\theta$$

Name_______________________________ ID#______________________________

For problems 1-7, pick all that is correct (similar to your Test-your-knowledge exercises in the HWs; Note that there will be **negative grading** for wrong answers.

1. In materials characterization, the probe and signal radiations (2 points)
   (a) Are the same
   (b) Are different
   (c) May be the same or may be different

2. Vibrational modes of any molecule (2 points)
   (a) are continuous in energy
   (b) are quantized in energy
   (c) can be used to probe the spring constant or the strength of the bond

3. When we rotate a crystal for a diffraction experiment (2 points)
   (i) The reciprocal lattice remains fixed/unchanged in the laboratory frame of reference
   (ii) The reciprocal lattice attached to the crystal rotates in the laboratory frame of reference
   (iii) The angle between the incident beam and any reciprocal lattice vector does not vary

4. H and He cannot be detected by Auger Electron Spectroscopy because (2 points)
   (i) No one has tried to do so?
   (ii) It is too expensive to make suitable samples
   (iii) Their electronic structure does not allow such non-radiative decay.

5. [1/3 ½ 1] and [2 3 6] refer to (2 points)
   (i) two different planes
   (ii) the same line
   (iii) a family of parallel planes passing through the origin.

6. It is best to use (2 points)
   (i) PES to probe filled levels in the valance bands
   (ii) inverse PES to probe unfilled levels in the conduction band
   (iii) XAS to probe unoccupied levels

7. The **maximum** number of electrons in the *L*-shell (n =2) is (2 points)
   (i) 4
   (ii) 6
   (iii) 20
   (iv) 8
   (v) 14

8. The three broad categories of techniques for materials characterization are (6 points)

   (a) _____ ____________________

   (b) __________ _____________________

Name________________________________ ID#_______________________________

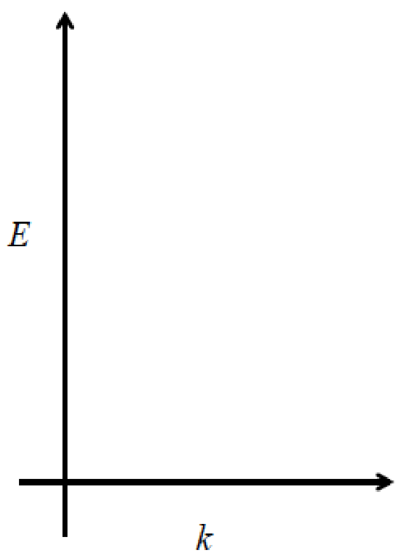
(c) ___________ _____________________

9. Plot the **Energy** (E) vs. **Wave-vector** (k) for (10 points)

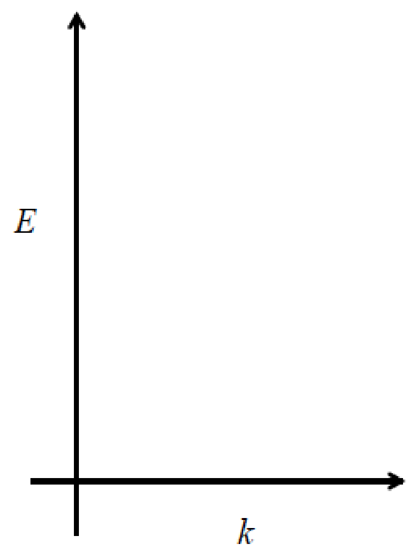
(a) **A free particle** of mass, m, whose energy is entirely **kinetic**.

(b) An electromagnetic wave **traveling in vacuum**

(a)



(b)



Name________________________________ ID#______________________________

10. For the Na atom, the binding energies of the various electrons are –1.071 keV (1*s*), –63.4 eV (2*s*), –30.7 eV (2*p*) and –5.14 eV(3*s*).

(a) Calculate the energy of the **K_α X-ray** line for Na. (5 points)

(b) If 1 eV = 1.6×10^{-19} J, $h = 6.62 \times 10^{-34}$ Js and $c = 3 \times 10^{8}$ m/s calculate the wavelength of this x-ray photon. (9 points)

(c) Can we use Na K_α for x-ray crystallography of real materials? Explain in a brief sentence or two. (6 points)

Name________________________________ ID#_______________________________

11. What is the **key difference** between (10 points)

(a) Infra-red and Raman Spectroscopies

(b) Rayleigh scattering and Raman spectroscopy

12. For **X-ray photoelectron spectroscopy**

The binding energy of a core-level of an **elemental metal**, work function ~ 5 eV, is –711 eV.

(i) If Al-K (~1486 eV) is used to probe this element at what energy of the photoelectron would the peak for this core-level appear in an XPS experiment, assuming $E_B = 0$ at the Fermi level? State your assumption clearly

(ii) Now, where would the peak appear if we assume $E_B = 0$ at the Vacuum level ?

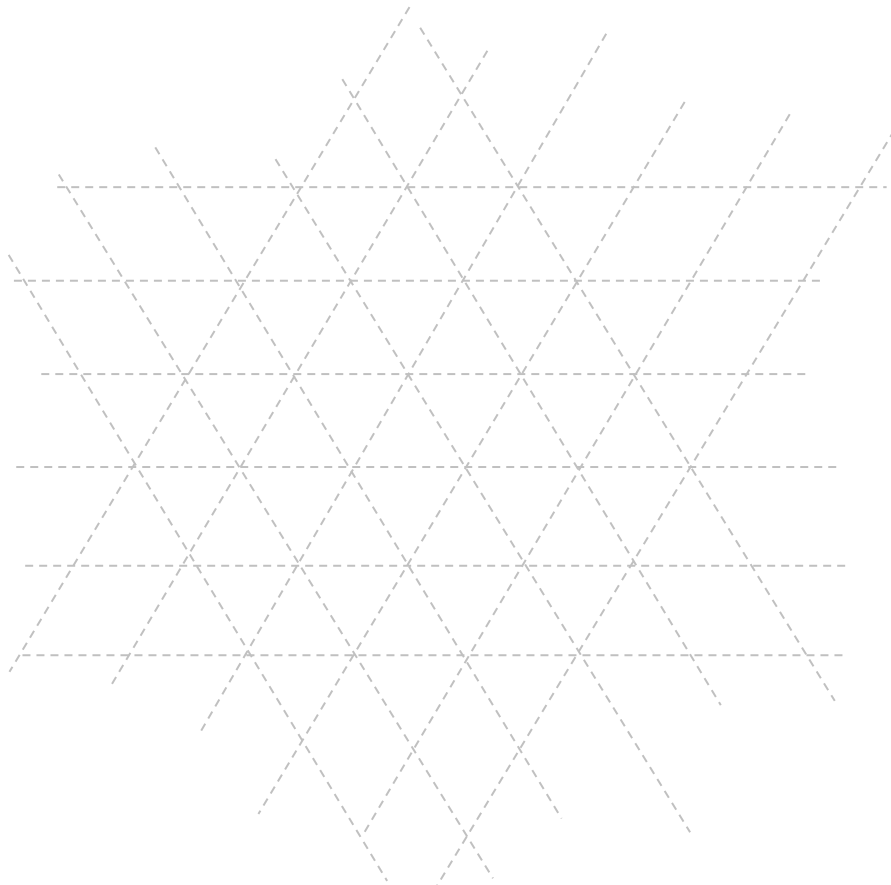
(iii) If we use Mg K (~1251 eV) instead, where would the peak appear in (i).

(10 points)

Name______________________________ ID#_____________________________

13. For a <u>two-dimensional</u> ***hexagonal*** unit cell, calculate its reciprocal lattice vectors. (hint: assume a hypothetical *c-axis* normal to the page). Draw the real lattice and the reciprocal lattice (label them clearly) on the same figure below. (10 points)

Name________________________________ ID#_______________________________



Name________________________________ ID#_______________________________

14. BONUS Question (10 points)

(a) What is Law of diffraction in **reciprocal space** ? Show it in a figure and define/describe all the variables.

(b) How is this related to the Bragg Law in **real space** ? Illustrate this also with a figure.