GEBZE TECHNICAL UNIVERSITY
Department of Materials Science and Engineering

MSE 301 SOLID STATE PHYSICS FOR ENGINEERS

Midterm Exam

Name	: *"Answer Key"*
Student number	:

Academic year : 2018-2019

Semester : FALL

Date : 13.11.2018

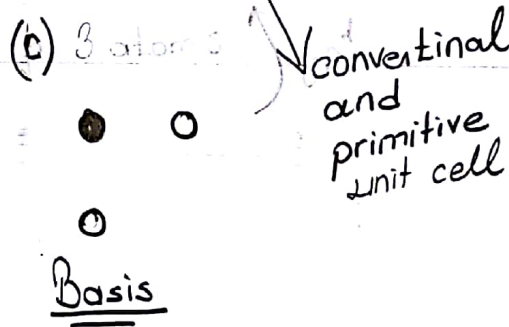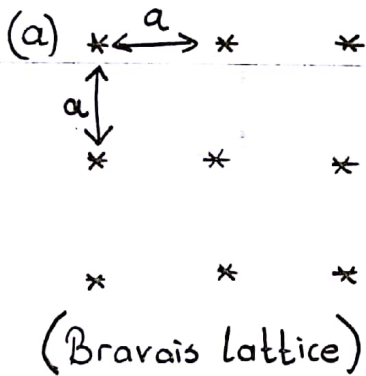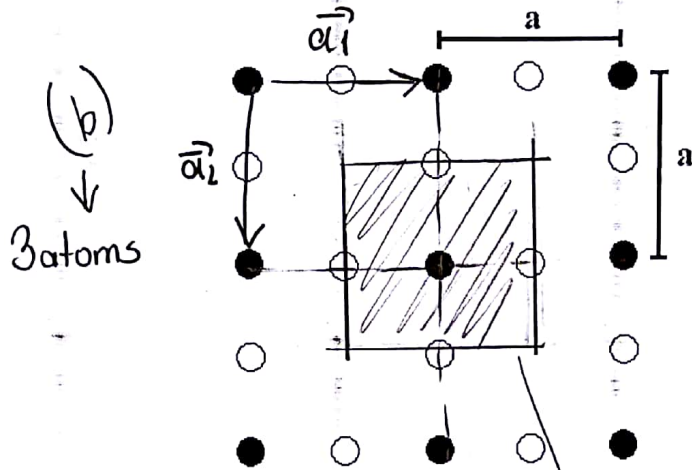Exam duration : 13.00-14:30

Instructor : Prof. Ebru MENŞUR-ALKOY

Question	1	2	3	4	5	6	Total
Points	15	20	20	15	20	10	100
Grade							

ALL QUESTIONS ARE MANDATORY!

1-) The common crystal structure view of copper oxide (CuO_2) in two-dimensional (2D) plane is shown in figure. The distance between copper atoms (filled circles) is "a".

15p

   a) Sketch the Bravais lattice in 2D.

   b) Indicate a possible set of primitive vectors in this plane. How many atoms are there in the primitive unit cell?

   c) What is the conventional unit cell and basis for this crystal?

Cu_2O

(b) $\vec{a_1}$ $\vec{a_2}$ 3 atoms

(a) a, a (Bravais lattice)

(c) 3 atoms   Basis   conventinal and primitive unit cell

2-) Answer these questions briefly: (each of 4 points)

a) How can you determine the structure of crystals?
b) Why do covalent crystals typically have a much lower packing density than metallic crystals?
c) Explain the difference between cohesive energy and lattice energy.
d) What typically happens when a crystal is exposed to a small stress?
e) What kind of elements are likely to form crystals through ionic bonding?

(a) By XRD, neutron diffraction methods.

(b) Because covalent bonding has directional nature.

(c) Cohesive energy is the energy required to seperate the components of a solid on infinite distance from each other. [no charge (atom)] Made of three parts: ① Coulomb int., ② from Pauli ex. principle and ③ from derived from quantum mechanics! Also called binding energy.

Lattice energy is for materials with ionic bonding and the energy required to seperate the ionic components.
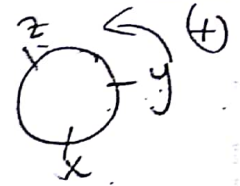
(d) $\sigma = \dfrac{F}{A}$ and $\varepsilon = \dfrac{\Delta \ell}{\ell}$ This region is in _elastic_ deformation.

This behaviour is _Linear_ and reversible for a strain. Hook's law is the corresponding law for that system. Force constant of the material is effective on that behavior ε.

→ Repulsive and attractive forces!

(e) Positive and negative ions form this bond. Electrostatic attractions are main mechanism. Electronegativities of these two ions is important for formation of this bond. Electronegativities must be different. Na^+ and Cl^- is the well-known example.

3-) 5   [20p]

a) What is the meaning and importance of reciprocal lattice for a crystal?
b) A Bravais lattice is specified by the primitive lattice vectors as given below:

$$\vec{a}_1 = a.\hat{x} \quad ; \quad \vec{a}_2 = \frac{a}{2}.\hat{x} + \frac{\sqrt{3}a}{2}.\hat{y} \quad ; \quad \vec{a}_3 := c.\hat{z}$$

Where $\hat{x}, \hat{y}, \hat{z}$ are unit vectors along x, y and z axes, respectively. a is the lattice constant.

5   b.1.) Make a sketch of the lattice in only x-y plane (2D). Indicate the nearest neighbours for a lattice points.

5   b.2.) Draw the Weigner-Seitz primitive cell for the lattice in the x-y plane.

5   b.3.) Find the primitive reciprocal lattice vector $\vec{b}_1$.

$$\tan\theta = \frac{\frac{\sqrt{3}\,a}{2}}{\frac{a}{2}} = \sqrt{3}$$
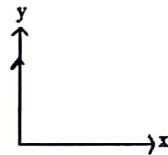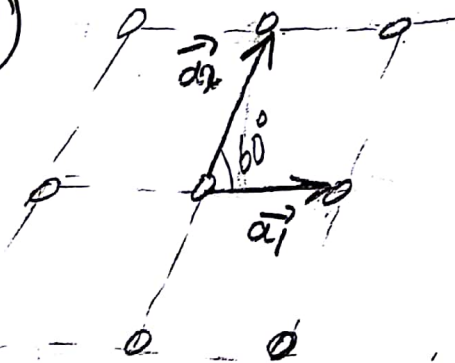
Hint:

$$V_C = \vec{a}_1.(\vec{a}_2 \times \vec{a}_3)$$

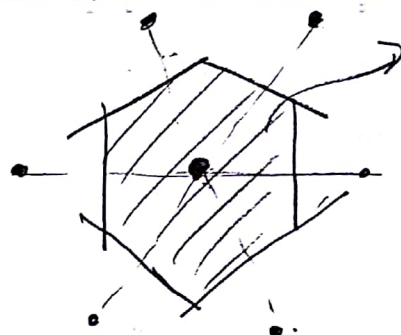$$\vec{b}_{i} = 2\pi.\left(\frac{\vec{a}_{i+1} \times \vec{a}_{i+2}}{V_C}\right)$$

$$\vec{G} = h.\vec{b}_1 + k.\vec{b}_2 + l.\vec{b}_3$$

$$\theta = 60° \; (\text{btw } x \text{ and } y \text{ axes})$$

(b.1)

(b.2)

Wigner-Seitz primitive cell in x-y

(b.3)

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

$$\vec{a}_2 \times \vec{a}_3 = -\hat{y}\left(\frac{a}{2}.c\right) + \hat{x}.\frac{\sqrt{3}.a}{2}.c$$

$$\vec{a}_1.(\vec{a}_2 \times \vec{a}_3) = \frac{\sqrt{3}.a^2}{2}.c = V$$

$$\vec{b}_1 = \frac{2\pi.a.c}{\frac{\sqrt{3}.a^2.c}{2}}\left(\hat{y}\left(\frac{-1}{2}\right) + \hat{x}.\frac{\sqrt{3}}{2}\right)$$

$$\vec{b}_1 = \frac{4\pi}{\sqrt{3}.a}\left(-\frac{\hat{y}}{2} + \frac{\hat{x}.\sqrt{3}}{2}\right)$$

4-) Answer the following questions on X-ray diffraction (XRD):

a) The Bragg condition is given as $2d.\sin\theta = n.\lambda$. What is the limit and relationship between d and λ for an instructive diffraction? Why?

b) Why do we use X-ray to determine crystal structure?

c) What is "<u>structure factor (S)</u>" of a crystal? What kind of parameters do we need to calculate the structure factor?

(a) $n\lambda = 2d\sin\theta$ Bragg condition. X-rays penetrate very deeply into the crystal so that thousands of layers contribute to the reflection. The Bragg condition can be fulfilled for $\boxed{\lambda < 2d}$, putting an upper limit on the wavelength of the X-rays that can be used for crystal structure determination.

(b) In order to explore the structure of the crystals, we require waves which interact with atoms and which have a wavelength comparable with the interatomic spacing in crystals; that is, we require a wavelength that is around nm level ($\sim 1nm$). This wavelength belongs to X-Ray in electromagnetic spectrum.

(c) The structure factor is a mathematical function describing the amplitude and phase of a wave diffracted from crystal lattice planes characterised by Miller indices h, k, l. $|F_{hkl}| = \dfrac{\text{Amplitude of the wave scattered by all atoms of}}{\text{Amplitude of wave scattered by one } e'}$

Thus all reflections that are allowed can be calculated.

To calculate SF, we should now atom coordinates (positions)

$$F_{hkl} = SF = \sum_{i=1}^{N} f_i \cdot e^{2\pi i (hu_i + kv_j + lw_i)}$$
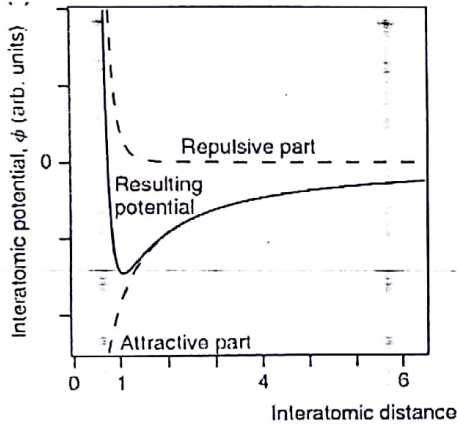$\hookrightarrow$ atomic factor!

5-) The typical potential energy ($\phi(x)$) versus interatomic distances (a) graph for two atoms is shown in figure. According to figure and the lecture:

<div style="text-align:right">20p</div>

a) Why is the interatomic potential graph is assymmetric?

b) What kind of physical properties do the curvature and the depth of this graph indicate? Explain each of it.

c) The interatomic force constant and other information about the crystal can be calculated from Taylor series as given below:

$$\phi(x) = \phi(a) + \frac{\phi'(a)}{1!}(x-a) + \frac{\phi''(a)}{2!}(x-a)^2 + \frac{\phi'''}{3!}(x-a)^3 + \ldots$$

Explain the meaning of the second and the third terms of this formula. Find the spring constant of K from the series.

d) Show the relationship between spring constant (K) and Young modulus (Y) for a material.

Interatomic potential, ϕ (arb. units)
Repulsive part
Resulting potential
Attractive part
Interatomic distance

(a) Because in repulsive and attractive forces are effective this interatomic potential. A simple expression of ϕ is written as $\phi(r) = \frac{A}{r^n} - \frac{B}{r^m}$ where r is the distance btw. atoms. Such a potential results with this graph.

(b) **Curvature** corresponds to thermal properties such as thermal expansion on the atomic scale. When T was increased the curvature of the graph will be change, because of the changing of the distance. Beside this curvature also means different linear restoring force of material. **Depth** is related to the bonding energy. Cohesive energy difference can be observed by depth of this graph.

(c) Second term is $\frac{d\phi(a)}{dx}$. This means equilibrium point (x=a) for this graph. Derivation equals to zero and this is the r or $\underline{x=a}$

Third term is $\frac{d^2\phi(a)}{dx^2}$. This is the harmonic potential linear force $K = \frac{d^2\phi(a)}{dx^2}$ Related to the curvature of the graph.

(d) $Y = \frac{\sigma}{\varepsilon} = \frac{F}{A} \cdot \frac{l}{\Delta l} \Rightarrow F = \left(\frac{Y \cdot A}{l}\right) \cdot \Delta l \quad \rightarrow$ Young modulus!
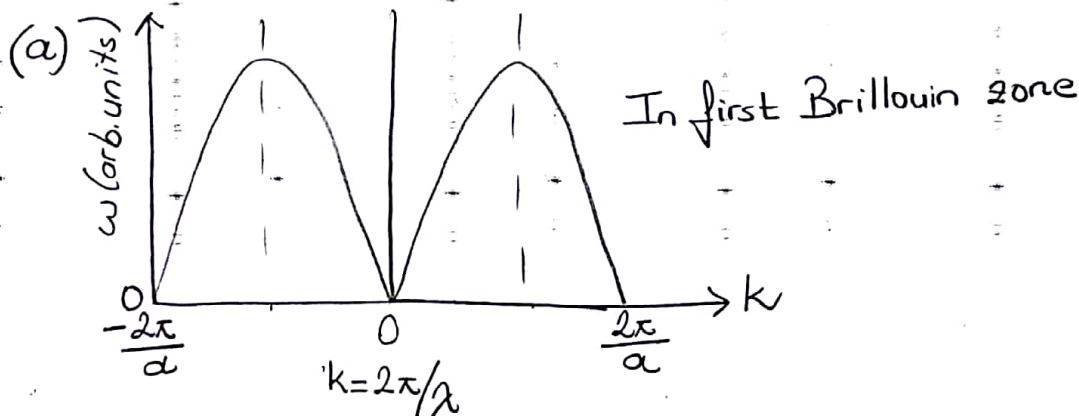
$K \rightarrow$ spring const.

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6-) The dispersion relation for the one dimensional chain (one atom per unit cell) can be given as: **10p**

$$\omega(k) = 2.\sqrt{\frac{K}{M}} \cdot \sin\left(\frac{k.\alpha}{2}\right)$$

Where K is the spring constant and k is the wave number.

a) Sketch the frequency (ω) graph in terms of wave number k.
b) Why do we need these periodic sinus function for decribing dispersion of ω?
c) If each unit cell contains __two atoms__, what kind of additional properties will be observed?

(a)

In first Brillouin zone

$k = 2\pi/\lambda$

(b) Equation of motion forasimple harmonic oscillator can be written as:

$$M\frac{d^2x}{dt^2} = -K.x \quad \text{and solution } x(t) = A.\cos(\omega t + \delta) \text{ and } \omega = \sqrt{\frac{K}{M}}$$
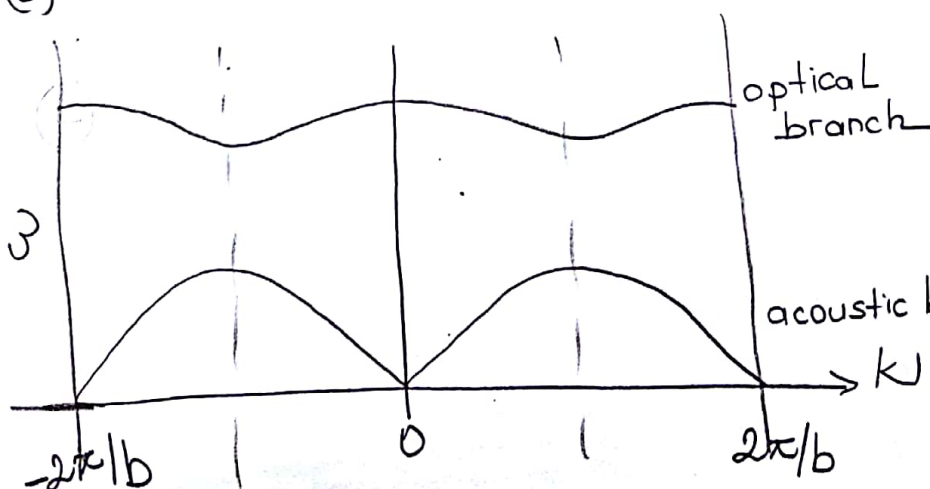
But for the periodic lattice' motion

$$M\frac{d^2U_n}{dt^2} = -K(U_n - U_{n-1}) + K(U_{n+1} - U_n)$$

$$\omega(k) = 2\sqrt{\frac{K}{M}} \cdot \sin\frac{ka}{2}$$

This is the dispersion relation and this sinus function shows the periodic behavior of the lattice motion

(c)

optical branch

acoustic branch

Optical modes can be induced by E-field)

$E = h.f$

$f \sim 10^{12} N_z$