

## Solid State Physics -1

### 1- Course Plan

- a. **Course Introduction and Outcomes:** Condensed Matter Physics is a core course for MSc (Physics) students. This course contains classification and properties of condensed or solid state materials, which can be explained on the basis of arrangement of atom, ions and electron motion, spin *etc.* The main objective of this course is to learn about properties and their response to internal and external stimuli. This goal can be achieved by learning crystal structure, crystal binding, lattice dynamics, electron, electron distribution theories and the concept of energy bands. The quantum and statistical mechanics concepts and formalisms are frequently used to understand the above features in condensed or solid materials.

b. **Course information**

Course title	Condensed matter physics
Department	Physics
Course type	Core
Program level	MSc
Contact hours	45
Facilities required	Class room, computers with internet facility

c. **Prerequisite**

Students' should be able to

- 1- Formulate and solve differential equations and calculate integrals with proper limits for a given scenario.
- 2- Construct and solve time dependent and time independent Schrodinger's wave equation for different situations and derive corresponding wave functions.
- 3- Explain and apply the Maxwell Boltzmann, Fermi Dirac and Boson-Einstein statistics for given scenarios and solve the problem
- 4- Write and solve matrixes, vector and tensors algebra.
- 5- Apply different quantum mechanical operators to different functions and solve them.
- 6- Apply the different electromagnetic theories and principle to given scenarios and solve the problem
- 7- Apply the statistical physics theories and principle to given scenarios and solve the problem

d. **Course outcome of the course**

- 1- Students will be able to **analyze** different types of matter depending on nature of chemical bonds and their properties
- 2- Students will be able **analyze** the crystal structures by **applying** crystallographic parameters.
- 3- Students will be able to determine the crystal structure by **analysis** of XRD data
- 4- Students will be able to **evaluate** and **analyze** the electrical and optical properties of solids
- 5- Students will be able to **analyze** electron transport and energy related problems by applying quantum mechanical principles
- 6- Students will be able to **analyze** the lattice vibration phenomenon in the solids

e. **Mapping of CO with Syllabus**

SNo	CO	Number of classes	Marks	Syllabus topics
1-	Students will be able to <b>analyze</b> different types of matter depending on nature of chemical bonds and their properties	7	16	Classification of solids and matter: crystalline, non-crystalline, nano-phase solids, liquids. Macroscopic description of condensed matter. Type of bonding, Ionic crystals, van der Waals bonds, . Covalent and metallic bonds
2-	Students will be able <b>analyze</b> the crystal structures by <b>applying</b> crystallographic parameters.	7	18	Crystal structure, Bravais lattices, Crystal system, unit cell, Miller indices, reciprocal lattice
3-	Students will be able to determine the crystal structure by <b>analysis</b> of XRD data	5	8	X-ray, neutron, electron diffraction. Bragg's law in direct and reciprocal lattice. Structure factor. Diffraction techniques.
4-	Students will be able to <b>analyze</b> the lattice vibration phenomenon in the solids	10	22	Lattice dynamics, harmonic oscillations, Dispersion relation, Summerfield theory, phonons for one- dimensional Mono-atomic and Diatomic linear lattices, Physical difference between optical and acoustic branches
5-	Student will be able to <b>apply the theory</b> for the	6	18	Electric, optical, thermal conductivity properties of solids,



## Assessment Plan for LO-1

Type of assessment	Frequency of assessment	Delivery from the learner	Data collection	Learning Verification	Decision making
Formative	After achieving LO	Team based learning (appendix)	Online questions (MCQ) by Learning management system (LMS)	Written/ verbal feedback to each student	
Summative	Quiz I, after 12-15 lectures	Test paper I	Hard copy	Evaluate the hard copy and grade	

### Example question for formative assessment

- If the repulsive energy is of the form  $Ce^{-r/a}$ , determine  $C$  and  $a$  for NaCl if the cohesive energy/ion pair is 6.61 eV, and the interatomic separation is 0.282 nm. Given that the ionisation energy of Na is 5.138 eV and the electron affinity of  $\text{Cl}^{-1}$  is 3.61 eV.

- $63.22 \times 10^3$
- $6.322 \times 10^3$
- $63.22 \times 10^{-3}$
- $6.322 \times 10^{-3}$

- The total energy of an ionic solid is given by an expression  $E = \frac{\alpha e^2}{4\pi\epsilon_0 r} + \frac{B}{r^9}$  where  $\alpha$  is Madelung constant,  $r$  is the distance between the nearest neighbours in the crystal and  $B$  is a constant. If  $r_0$  is the equilibrium separation between the nearest neighbours then the value of  $B$  is

- $\frac{\alpha e^2 r_0^8}{36\pi\epsilon_0}$
- $\frac{\alpha e^2 r_0^8}{4\pi\epsilon_0}$
- $\frac{2\alpha e^2 r_0^{10}}{9\pi\epsilon_0}$
- $\frac{\alpha e^2 r_0^{10}}{36\pi\epsilon_0}$
- 

- The potential of a diatomic molecule as a function of the distance  $r$  between the atoms is given by  $V(r) = \frac{a}{r^6} + \frac{b}{r^{12}}$ . The value of the potential at equilibrium separation between the atoms is:

- $-4a^2/b$
- $-2a^2/b$
- $-a^2/2b$

d.  $-a^2/4b$

4. In an insulating solid which one of the following physical phenomena is the consequence of the Pauli's exclusion principle?
- Ionic conductivity
  - Ferromagnetism
  - Para magnetism
  - Ferroelectricity
5. The solid phase of an element follows van-der-Waals bonding with inter-atomic potential  $V(r) = \frac{P}{r^6} + \frac{Q}{r^{12}}$  where, P and Q are constants. The bond length can be expressed as
- $\left(\frac{2Q}{P}\right)^{-6}$
  - $\left(\frac{Q}{P}\right)^{-6}$
  - $\left(\frac{Q}{2P}\right)^{-6}$
  - $\left(\frac{P}{Q}\right)^{-6}$
6. Why are the glass panels installed on buildings not transparent?
- Because of unwanted deposits
  - Because it becomes old
  - Because it is brittle
  - Because of a thin coating*
7. Which of the following is a crystalline solid?
- Anisotropic substances*
  - Isotropic substances
  - Super cooled liquids
  - Amorphous solids
8. The degree of freedom at triple point in unary phase diagram for water is \_\_\_\_\_
- 2
  - 3
  - 0
  - 1

### Example questions for summative questions

- 1- Develop a new form of equation for the potential energy of a pair of atom or molecules from the equation

$$U(r) = -\frac{a}{r^m} + \frac{b}{r^n}$$

Determine from this equation, expressions for (a) potential energy at  $r = r_0$  ( $U_{\min}$ ); (b) the spacing at the points of inflection.

- 2- Assume the energies of two particles in the field of each other is given by the function  $U(r) = -(a/r) + (b/r^8)$ , where a and b are constants and r is the distance between the centres of the particles.

Show that if the particles are pulled apart, the bond will break as soon as

$$r = \left[ \frac{36b}{a} \right]^{1/7} = r_0 4.5^{1/7}$$

- 3- (a) Determine the inter-ionic equilibrium distance between the sodium and chlorine ions in a sodium chloride molecule if the bond energy is 3.84 eV and the repulsive exponent is 8.

(b) At the equilibrium distance, how much (in percent) is the contribution to the attractive bond energy by electron shell repulsion?

- 4- Consider a 100 Watt bulb emitting light in all directions. Suppose that a metallic sodium surface is kept at a distance of 1 m from the bulb. Estimate the time needed by an electron in an Na atom to receive an energy of 1 eV. Assume that all the energy is absorbed by the top layer of the surface and all the energy absorbed by an Na atom is taken up by one electron.

- 5- Consider the three physical states of matter; rank them in ascending order of kinetic energy of the molecules/atoms; repeat the same for potential energy.

- 6- The binding energy per molecule of NaCl is 7.95 eV. The repulsive term of the potential is of the form  $K/r^9$ , where K is a constant. The value of the Madelung constant is.....(up to three decimal place)

- 7- The unit cell parameter of NaCl is 5.56 Å and the modulus of elasticity along [100] direction is  $6 \times 10^{10}$  N/m<sup>2</sup>. Estimate the wavelength at which an electromagnetic radiation is strongly reflected by the crystal. At. Wt. of Na=23 and of Cl=37.

#### Resources:

- 1- <http://stp.clarku.edu/simulations/>
- 2- <https://ocw.mit.edu/courses/materials-science-and-engineering/3-091sc-introduction-to-solid-state-chemistry-fall-2010/bonding-and-molecules/self-assessment/>

CO 2: Students will be able **analyze** the crystal structures by **applying** crystallographic parameters.

S.No.	LO	Pedagogical Decision	Brief Description	Sample Technology
2	Draw Find Calculate Compute Determine	ACL (Active Cooperative Learning)  Scaffolding for problem solving (appendix)	<b>Teacher:</b> Provides worksheet for Applets and numerical problems (based on applet and LO) <b>Student:</b> will work in group and groups will evaluate and comment on each other's solution with teacher's involvement	Technology: Applet with worksheet, PPT LMS: Formative assessment and students' feedback

#### Assessment Plan for LO-2

Type of assessment	Frequency of assessment	Delivery from the learner	Data collection	Learning Verification	Decision making
<b>Formative</b>	After achieving LO	MCQ	Online MCQ LMS	Formal written feedback /verbal feedback	
<b>Summative</b>	Quiz I, after 15-18 classes	Test paper I	Hard copy	Evaluate the hard copy and grade Weightage for this portion: 25 %	

#### Resource

- <http://escher.epfl.ch>
- <http://www.jcrystal.com/steffenweber/java.html>
- <http://www.webmineral.com/crystall.shtml#.XGKKHC-B10>

#### Example questions for formative assessment

- The structure factor of a single cell of identical atoms of (form factor  $f$ ) is given by  $S_{hkl} = f \sum \exp[-2\pi i(x_j h + y_j k + z_j l)]$ , where  $(x_j, y_j, z_j)$  is the coordinate of an atom, and  $h, k, l$  are Miller indices. Each of the following options represent allowed diffraction peaks from the corresponding set of planes in FCC and BCC structures. Which one of the following statement is correct?
  - Bcc : (200);(110);(222)      fcc: (111);(311);(400)
  - Bcc : (210);(110);(222)      fcc: (111);(311);(400)
  - Bcc : (200);(110);(222)      fcc: (111);(211);(400)
  - Bcc : (200);(210);(222)      fcc: (111);(211);(400)
- Metallic monovalent sodium crystallizes in body centred cubic structure. If the length of the unit cell is  $4 \times 10^{-8}$  cm, the concentration of conduction electrons in metallic sodium is

- a.  $6.022 \times 10^{23} \text{ cm}^{-3}$
- b.  $3.125 \times 10^{22} \text{ cm}^{-3}$
- c.  $2.562 \times 10^{21} \text{ cm}^{-3}$
- d.  $1.250 \times 10^{20} \text{ cm}^{-3}$

3- A lattice has the following primitive vectors (in Å)  $\vec{a} = 2(i + j)$ ,  $\vec{b} = 2(k + j)$ ,  $\vec{c} = (i + j)$ . The reciprocal lattice corresponding to the above lattice is

- a. BCC lattice with cube edge of  $\left(\frac{\pi}{2}\right) \text{ \AA}^{-1}$
- b. BCC lattice with cube edge of  $(2\pi) \text{ \AA}^{-1}$
- c. FCC lattice with cube edge of  $\left(\frac{\pi}{2}\right) \text{ \AA}^{-1}$
- d. FCC lattice with cube edge of  $(2\pi) \text{ \AA}^{-1}$

4- The Miller indices of a plane passing through the three points having coordinates  $(0,0,1)$ ,  $(1,0,0)$ ,  $(1/2,1/2, 1/4)$  are

- a.  $(2,1,2)$
- b.  $(1,1,1)$
- c.  $(1,2,1)$
- d.  $(2,1,1)$

5- If the ionic radii of Mn and S are 0.80 and 1.84 nm respectively, the structure of MnS will be

- a. Cubic close pack
- b. Primitive cubic cell
- c. *Body centred cubic*
- d. NaCl type

6- Consider the atomic packing factor (APF) of the following lattices

- I. Simple cubic
- II. Body centred cubic
- III. Face centred cubic
- IV. Hexagonal close packed

Which two of the above structures have equal APF?

- a. I and II
- b. III and IV
- c. I and III
- d. *II and IV*

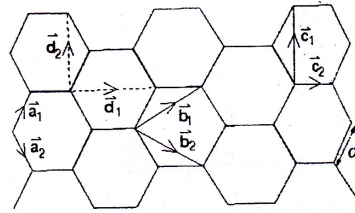
7- For a closed packed BCC structure of hard spheres, the lattice constant  $a$  is related to the sphere radius  $R$  as

- a.  $a = 4R \sqrt{3}$
- b.  $a = 2R \sqrt{3}$



- c.  $a = 2R\sqrt{2}$
- d.  $a = 4R\sqrt{2}$

8- The two dimensional lattice of graphene is an arrangement of Carbon atoms forming a honeycomb structure of lattice spacing  $a$ , as shown below. The carbon atoms occupy the vertices.



(A) The Wigner-Seitz cell has an area of

- a.  $2a^2$
- b.  $\sqrt{\frac{3}{2}}a^2$
- c.  $6\sqrt{3}a^2$  (d)
- d.  $3\sqrt{3}a^2$

(B) The Bravais lattice for this array is a

- a. Rectangular lattice with basis vectors  $d_1$  and  $d_2$
- b. Rectangular lattice with basis vectors  $c$  and  $c$
- c. Hexagonal lattice with basis vectors  $a_1$  and  $a_2$
- d. Hexagonal lattice with basis vectors  $b$  and  $b_{12}$

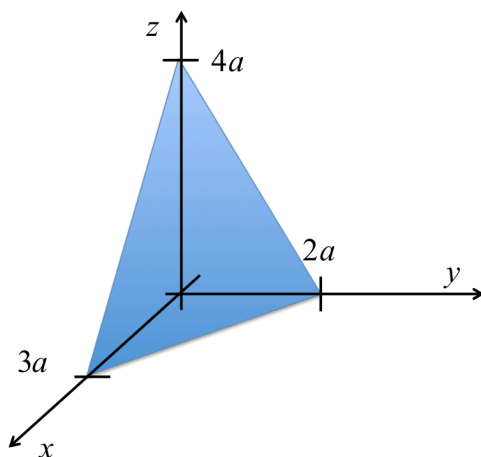
9- The vector direction normal to the plane (110) is:

- a. [001]
- b. [010]
- c. [100]
- d. [011]
- e. [110]

### Example questions for summative assessment

1. Show that the maximum radius of the sphere that can just fit into the void at the body centre of the *fcc* structure coordinated by the facial atom is  $0.414r$ , where  $r$  is the radius of the atom.

2. Draw a unit cell of the NaCl crystal. Describe the structure in terms of a lattice and a motif. What is the kind of bonding in the solid? Calculate the packing fraction. Is this a close packed structure?
3. Compute the atomic density of (100), (110) and (111) planes in SC, BCC, FCC crystals. Include only those atoms whose centre of mass lies on the plane.
4. Atom, which can be assumed to be a hard sphere of radius  $R$ , is arranged in FCC lattice with lattice constant  $a$ , such that each atom touches its nearest neighbours. Take the centre of the radius  $r$  (assumed to be hard sphere) is to be accommodate at the position  $(0, a/2, 0)$  without distorting the lattice. The maximum value of  $r/R$  is.....
5. Determine following parameters for the given Fig.
  - a. Determine the Miller indices of the plane sketched below
  - b. Determine the direction normal to the plane
  - c. Determine the spacing between equivalent planes of this kind (in terms of the lattice spacing,  $a$ )
  - d. Determine the angle between this plane and a (100) plane.



6. Molybdenum (Mo) crystallizes in a body-centered cubic structure with a lattice constant of  $a = 3.147$  Angstroms. Answer the following questions about Mo.
  - a. Compute the number of Mo atoms per  $\text{cm}^3$ .
  - b. Compute the center-to-center spacing of nearest neighbour Mo atoms in Angstroms.
  - c. Assuming that the radius of a Mo atom is one-half the center-to-center spacing of nearest neighbours, compute the percent of the cubic volume,  $a^3$ , that is occupied by Mo atoms.
  - d. Compute the surface density of Mo atoms on a (110) plane in number per  $\text{cm}^2$ .

CO 3: Students will be able to determine the crystal structure by **analysis** of XRD data

S.No.	LO-3	Pedagogical Decision	Brief Description	Sample Technology
3	Determine Find Calculate Compute Explain	<b>Hands on experience</b> (Experiment in X ray lab) and lecture	<b>Teacher:</b> Lab visit (how X ray works); Lecture by teacher on data analysis <b>Students:</b> Experimental data collection and analysis	XRD facility, Computer
		Problem solving Scaffolding	<b>Teacher:</b> ask students to write all the formula from concept. Then find out which one or combinations will be applied to solve a given problem <b>Students:</b> will follow the teacher's instructions and solve the numerical/problems	

### Assessment Plan For LO-3

Type of assessment	Frequency of assessment	Delivery from the learner	Data collection	Learning Verification	Decision making
<b>Formative</b>	After lab visit	Report on lab visit by each student	Hard or soft copy by LMS	Written feedback on report	
	After achieving LO or after few classes	MCQ	Verbal in class OR by LMS or online	Verbal feedback during class Or written feedback by LMS	
<b>Summative</b>	Quiz I , after 15-18 classes	Test paper I	Hard copy	Evaluate and grade the hard copy ; Weightage for this portion: 25 %	

### Resources

- 1- <https://myscope.training>

2- <https://nanohub.org/groups/ece305s1>

### Example questions for formative assessment

1- Consider X-ray diffraction from a crystal with a face centred cubic lattice. The lattice plane for which there is no diffraction peak is

- a. (2,1,2)
- b. (1,1,1)
- c. (2,0,0)
- d. (3,1,1)

2- The distance between the adjacent planes in  $\text{CaCO}_3$  is 0.3 nm. The smallest angle of Bragg's scattering for 0.03 nm X-ray is (*apply*)

- a.  $2.9^\circ$
- b.  $1.5^\circ$
- c.  $5.8^\circ$
- d.  $0.29^\circ$

3- If the (0 0 2) planes diffract at ( 2 theta or theta )  $60^\circ$ , then lattice parameter is

- a. 2.67 Å
- b. 3.08 Å
- c. 3.56 Å
- d. 5.34 Å

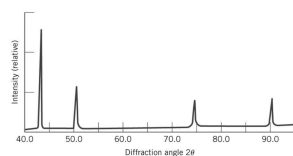
4- The NaCl crystal has the cell-edge  $a = 0.563$  nm. The smallest angle at which Bragg reflection can occur corresponds to a set of planes whose indices are

- a. (1 0 0)
- b. 1 1 0
- c. 1 1 1
- d. 2 0 0

### Example questions for summative assessment

1- Figure (below) shows the first four peaks of the x-ray diffraction pattern for copper, which has an FCC crystal structure; monochromatic x-radiation having a wavelength of 0.1542 nm was used.

- a. Index (i.e., give h, k, and l indices) for each of these peaks.
- b. Determine the interplanar spacing for each of the peaks.
- c. For each peak, determine the atomic radius for Cu and compare these with the values presented in the data



- 2- Rajni Sharma conducted an experiment with her X-ray diffractometer. A specimen of the Tantalum (Ta) is exposed to a beam of monochromatic x-ray of wavelength set by the  $K_{\alpha}$  line of titanium (Ti). Calculate the value of the smallest Bragg angle,  $\theta_{hkl}$  at which Rajni can expect reflection from the Ta specimen

Hint: The smallest  $\theta$  is associated with the largest d spacing ( $\lambda = 2d\sin\theta$ )

- 3- Calculate the acceleration potential that will result in electron diffraction from the (311) plane of platinum (Pt) at an angle  $\theta$  of  $33.3^{\circ}$ . The lattice constant of platinum,  $a$ , has a value of  $3.92 \text{ \AA}$ . (CO-3)
- 4- If you wanted to increase the angle at which the reflection described in part (a) is observed, would you replace the Mo target with a silver (Ag) target or a copper (Cu) target? Explain the reasoning behind your choice. (understanding/analyse)
- 5- A Debye-Scherrer powder diffraction experiment using incident copper (Cu)  $K_{\alpha}$  radiation resulted in the following set of reflections expressed as at the following values of  $2\theta$ :  $38.40^{\circ}$ ,  $44.59^{\circ}$ ,  $64.85^{\circ}$ ,  $77.90^{\circ}$ ,  $81.85^{\circ}$ ,  $98.40^{\circ}$ ,  $11.20^{\circ}$
- Determine the crystal structure
  - Calculate the lattice constant,  $a$ .
  - Assume that the crystal is a pure metal and on the basis of the hard-sphere approximation, calculate the atomic radius.

CO 4: Students will be able to **evaluate** and **analyze** the electrical and optical properties of solids.

S.No.	LO-4	Pedagogical Decision	Brief Description	Sample Technology
4	Compare	Project/ problem Based Learning OR	Explained below	Computer
	Calculate Choose Justify Determine Draw	Guided inquiry with scaffolding	The teacher provides a question to a group of students. Students will propose a solving method. The teacher can observe and provide feedback to groups if needed. Students interpret the known concepts and their inquiry questions and summarize their findings. The teacher can evaluate the team performance through	

		Problem solving by Peer instruction	different formative assessments.  Teacher : Teacher will provide the problem Students: will solve problem first individually and then in groups. Process will be followed by classroom discussion	
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#### Assessment Plan for LO-4

Type of assessment	Frequency of assessment	Delivery from the learner	Data collection	Learning Verification	Decision making
<b>Formative</b>	After achieving LO	Presentation by group and peer evaluation	Hard copy	Marks with feedback/ verbal feedback	
	Every week	Discussion with teams	Progress of the work	Verbal Feedback	
<b>Summative</b>	Quiz II, after 33-36 classes	Test paper II	Hard copy	Evaluate and grade the hard copy; Weightage 25 %	

#### Resources

- 1- <http://ee.sharif.edu/~sarvari/solidstate/solidstate.html>
- 2- [https://ocw.mit.edu/courses/materials-science-and-engineering/3-091sc-introduction-to-solid-state-chemistry-fall-2010/electronic-materials/13-band-theory-of-solids/MIT3\\_091SCF09\\_hw13\\_sol.pdf](https://ocw.mit.edu/courses/materials-science-and-engineering/3-091sc-introduction-to-solid-state-chemistry-fall-2010/electronic-materials/13-band-theory-of-solids/MIT3_091SCF09_hw13_sol.pdf)

**Assessment Rubrics (Presentation and peer evaluation) are attached in the appendix**

**Example of problem:** Optical properties of materials

#### Problem/project based learning:

Problem 1: Mr. X was facing the problem of high electric bill for his office. He consulted the staff and found that electricity bill can be reduced by using sunlight for office lighting. Mr. X contacted to a glass making company. He wanted to design an office room for him in which sunlight can replace electric lighting and the intensity can also be adjusted. Your team has to find out the design (coating material on glass) of glass suitable for his office room.

Problem 2: Suggest modification to glass coating to get maximum conductivity with highest transparency. (scaffolding)

**Students' role:**

- 1- Analyze the problem and find out the objectives
- 2- Identify the learning target
- 3- Prepare work plan and team work plan (separate table can provide with group members' names and date)
- 4- Material you want
- 5- Evidence of success for each

**Teacher's Role**

- 1- Teacher will provide problem/project to each group (4-5 students each group)
- 2- Teaching plan

Knowledge and skill needed	Students already know	Teacher has to teach before giving problem	Teacher has to teach during problem solving

**Example questions for Formative assessment**

1. The electrical conductivity of copper is approximately 95% of the electrical conductivity of silver, while the electron density in silver is approximately 70% of the electron density in copper. In Drude's model, the approximate ratio ( $\tau_{Cu}/\tau_{Ag}$ ) of the mean collision time in copper ( $\tau_{Cu}$ ) to the mean collision in ( $\tau_{Ag}$ ) is
  - a. 0.44
  - b. 1.50
  - c. 0.33
  - d. 0.66
  
2. Consider a one-dimensional chain of the atoms with lattice constant  $a$ . the energy of an electron with wave vector  $k$  is  $\epsilon(k) = \mu - \gamma \cos(ka)$ , where  $\mu$  and  $\gamma$  are constants. If an electric field  $E$  is applied in the positive  $x$  direction, the time dependent velocity of an electron is ( $B$  is a constant)
  - a. Proportional to  $\cos\left(B - \frac{eE}{\hbar} at\right)$
  - b. Proportional to  $E$
  - c. Independent of  $E$
  - d. Proportional to  $\sin\left(B - \frac{eE}{\hbar} at\right)$

3. The atomic density of a solid is  $5.85 \times 10^{28} \text{ m}^{-3}$ . Its electric resistivity is  $1.6 \times 10^{-8} \Omega\text{-m}$ . Assume that electrical conduction is described by the Drude model (classical theory), and that each atom contributes one conduction electron. The drift mobility (in  $\text{m}^2\text{N-s}$ ) of the conduction electron is
- $6.67 \times 10^{-3}$
  - $6.67 \times 10^{-6}$
  - $7.63 \times 10^{-3}$
  - $7.63 \times 10^{-6}$
4. (Using the data from previous question) the relaxation time (~~mean-free-path~~) in second of the conduction electrons is
- $3.98 \times 10^{-15}$
  - $3.79 \times 10^{-14}$
  - $2.84 \times 10^{-12}$
  - $2.64 \times 10^{-11}$
5. An intrinsic semiconductor with mass of hole  $m_h$ , and the mass of electron  $m_e$  is at a finite temperature  $T$ . If the top of the valance band energy is  $E_v$  and the bottom of the conduction band energy is  $E_c$ , the Fermi energy of the semiconductor is
- $E_f = \left(\frac{E_v + E_c}{2}\right) - \frac{3}{4} k_B T \ln\left(\frac{m_h}{m_e}\right)$
  - $E_f = \left(\frac{k_B T}{2}\right) + \frac{3}{4} (E_v + E_c) \ln\left(\frac{m_h}{m_e}\right)$
  - $E_f = \left(\frac{E_v + E_c}{2}\right) + \frac{3}{4} k_B T \ln\left(\frac{m_h}{m_e}\right)$
  - $E_f = \left(\frac{k_B T}{2}\right) - \frac{3}{4} (E_v + E_c) \ln\left(\frac{m_h}{m_e}\right)$
6. A thin metal film of dimension  $2 \text{ mm} \times 2 \text{ mm}$  contains  $4 \times 10^{12}$  electrons. The magnitude of the Fermi wavevector of the system, in the free electron approximation, is
- $2\sqrt{\pi} \times 10^7 \text{ cm}^{-1}$
  - $\sqrt{2\pi} \times 10^7 \text{ cm}^{-1}$
  - $\sqrt{\pi} \times 10^7 \text{ cm}^{-1}$
  - $2\pi \times 10^7 \text{ cm}^{-1}$
7. A phosphorous doped silicon semiconductor (doping density:  $10^{17}/\text{cm}^3$ ) is heated from  $100^\circ\text{C}$  to  $200^\circ\text{C}$ . Which of the following statement is correct
- Position of the fermi level will move towards conduction band
  - Position of dopant level will toward conduction band
  - Position of Fermi level moves towards the middle of the energy gap
  - Position of dopant level moves towards the middle of energy gap



8. If minority carrier electrons are injected at the left face of a *p*-type semiconductor, and there is **significant recombination** in the semiconductor, and the right contact enforces equilibrium conditions (i.e.  $\Delta n = 0$ ), how does the steady-state minority electron profile,  $\Delta n(x)$ , vary with position?
- $\Delta n(x)$  decreases linearly with position from left to right.
  - $\Delta n(x)$  increases linearly with position from left to right.
  - $\Delta n(x)$  decreases as the square of distance from left to right.
  - $\Delta n(x)$  increases as the square of distance from left to right.
9. The Einstein Relation,  $D = \mu k_B T / q$  (symbols have their usual meaning) relates the mobility to the diffusion coefficient. Under what conditions is it valid?
- always
  - only at equilibrium or very near equilibrium
  - only for parabolic band semiconductors
  - only for direct gap semiconductors
  - only for indirect gap semiconductors
10. How do we determine the electric field vs. position,  $x$ , from an energy band diagram?
- The electric field is  $E_C(x)$ .
  - The electric field is  $E_V(x)$ .
  - The electric field is  $E_i(x)$ .
  - The electric field is obtained by flipping  $E_C(x)$  upside down.
  - The electric field is the slope of  $E_C(x)$ .
11. Comparing the electrical conductivity to the lattice thermal conductivity, which of the following statements is true?
- The electrical conductivity can be positive or negative, but the lattice thermal conductivity is always positive.
  - The lattice thermal conductivity varies over many orders of magnitude.
  - The electrical conductivity varies over many orders of magnitude.
  - The two are related by the Wiedmann-Franz Law.
12. Diffusion involves random thermal motion and scattering. If the thermal velocity is  $v_T$  and the average distance between electron (or hole) scattering events is  $\lambda$ , what is the diffusion coefficient in  $\text{cm}^2/\text{s}$ ?
- $D = v_T \lambda / 2$
  - $D = v_T / (2\lambda)$
  - $D = \lambda / 2 v_T$
  - $D = v_T \lambda^2 / 2$

### Example questions for summative assessment

- 1- An unknown material is transparent to light of frequencies ( $\nu$ ) up to  $1.3 \times 10^{14}$  Hz. Draw a band structure for this material demonstrating the above information.
- 2- A material exhibits an “optical band edge” (transition from absorption of light to transmission) at  $\nu = 5 \times 10^{14}$  Hz .
  - a. Draw a diagram which reflects the indicated optical behavior.
  - b. What do you expect the color of this material to be when viewed in daylight?
  - c. What is the band gap ( $E_g$ ) of this material?
- 3- Determine the degree of degeneracy of the energy level  $(38 h^2/8ma)^2$  of a particle in a cubical potential box of side  $a$ .
- 4- A pure crystalline material (no impurities or dopants are present) appears red in transmitted light.
  - a. Is this material a conductor, semiconductor or insulator? Give reasons for your answer .
  - b. What is the approximate band gap ( $E_g$ ) of this material in eV?
- 5- The donor concentration in a sample of  $n$ -type silicon is increased by a factor of 100. The shift in the position of the fermi level at 300 K, assuming the sample to be non-degenerated is ... ..(meV)
- 6- The number density of electrons in the conduction band of a semiconductor at a given temperature is  $2 \times 10^{19} \text{ cm}^{-3}$ . Upon lightly doping this semiconductor with donor impurities, the number density of conduction electrons at the same temperature become  $4 \times 10^{20} \text{ m}^{-3}$ . The ratio of majority to minority charge carrier concentration is .....
- 7- The band gap of an intrinsic semiconductor is  $E_g = 0.72 \text{ eV}$  and  $m_h = 7 m_e$ . At 300 K the Fermi level with respect to the edge of the valence band (in eV).....
- 8- What is the Debye frequency for Copper, if its Debye temperature is 315 K. Also find the Debye specific heat at 10 K and 300 K. (evaluate / analysis. thermal)

- 9- Consider the conduction band of Si. Typically, only the states near the bottom of the conduction band are occupied with electrons. Assume that all states within 0.1 eV of the bottom of the band are occupied. Answer the following questions:
- How many electrons are in the conduction band? Express your answer per  $\text{cm}^3$ .
  - Compare this number to the atomic density of Si.

**CO 5:** Students will be able to **analyze** electron transport and energy related problems by applying quantum mechanical principles

Sl. No.	LO-5	Pedagogical Decision	Brief Description	Sample Technology
5	Derive Solve Calculate Compute	ACL  Problem solving	<b>Teacher:</b> will provide worksheet based on applet; Give clear instruction to avoid ambiguity and set the rule for class. Monitor and guide as and when needed. <b>Students:</b> will solve worksheet in groups. Team performance will be evaluated through peer assessment, discussion between groups	Applet with computer  <a href="http://jas.eng.buffalo.edu/education/semicon/fermi/functionAndStates/functionAndStates.html">http://jas.eng.buffalo.edu/education/semicon/fermi/functionAndStates/functionAndStates.html</a>

#### Assessment plan for LO-5

Type of assessment	Frequency of assessment	Delivery from the learner	Data collection	Learning Verification	Decision making
<b>Formative</b>	After achieving Learning	Worksheet	Computer: LMS (Moodle/Edmodo)	Written Feedback on worksheet	
	Every class	Question during class	Verbal	Verbal feedback	
<b>Summative</b>	Quiz 2	Test Paper I	Hard copy	Evaluation and grading of hard copy Weightage : 25 %	

#### Assessment questions

**Formative** Worksheets are provided with applets, if teacher wants, can modify them

### Example questions for formative assessment

- 1- The energy gap and lattice constant of an indirect band gap semiconductor are 1.875 eV and 0.52 nm respectively. Assume the dielectric constant of the material to be unity. When it is excited by broadband radiation, an electron initially in the valence band at  $k = 0$  makes a transition to the conduction band. The wavevector of the electron in the conduction band, in terms of the wavevector  $k_{\max}$  at the edge of the Brillouin zone, after the transition is closest to

- a.  $k_{\max}/10$
- b.  $k_{\max}/100$
- c.  $k_{\max}/1000$
- d. 0

- 2- The band energy of an electron in a crystal for a particular  $k$ -direction has the form  $\varepsilon(k) = A - B\cos 2ka$ , where  $A$  and  $B$  are positive constants and  $0 < ka < \pi$ . The electron has a hole-like behaviour over the following range of  $k$ ;

- a.  $\frac{\pi}{4} < ka < \frac{3\pi}{4}$
- b.  $\frac{\pi}{2} < ka < \pi$
- c.  $0 < ka < \frac{\pi}{4}$
- d.  $\frac{\pi}{2} < ka < \frac{3\pi}{4}$

- 3- Consider electrons in graphene, which is a monoatomic layer of carbon atoms. If the dispersion relation of the electrons is taken to be  $\varepsilon(k) = ck$  (where  $c$  is constant) over the entire  $k$ -space, then the Fermi energy  $\varepsilon_f$  depends on the number density of electrons  $\rho$  as

- a.  $\varepsilon_f \propto \rho^{\frac{1}{2}}$
- b.  $\varepsilon_f \propto \rho$
- c.  $\varepsilon_f \propto \rho^{\frac{2}{3}}$
- d.  $\varepsilon_f \propto \rho^{\frac{1}{3}}$

- 4- A one-dimensional linear atomic chain contains two types of atoms of masses  $m_1$  and  $m_2$  (where  $m_2 > m_1$ ), arranged alternately. The distance between successive atoms is the same. Assume that the harmonic approximation is valid. At the first Brillouin zone boundary, which statement is correct ?

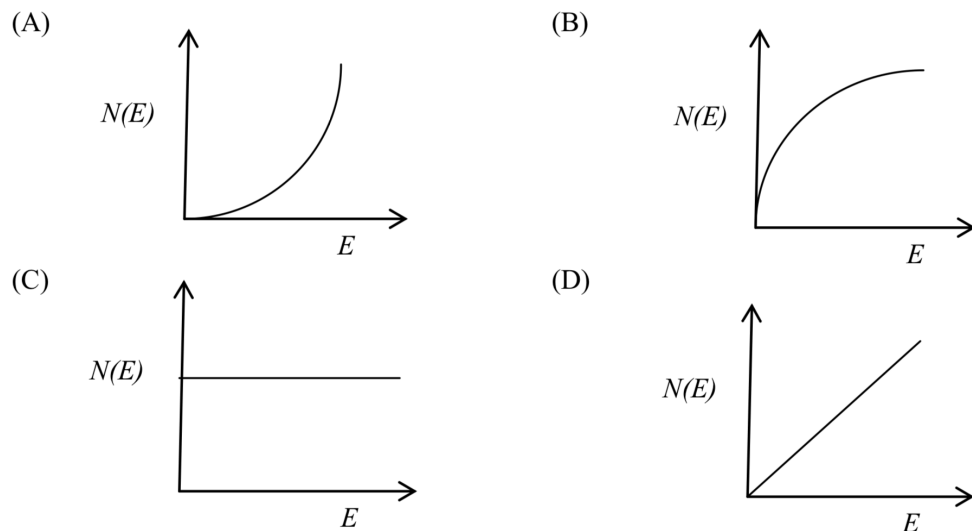
- a. The atoms with mass  $m_2$  are at rest in the optical mode, while they vibrate in the acoustical mode
- b. The atoms of mass  $m_1$  are at the rest in the optical mode, while they vibrate in the acoustical mode

- c. Both types of atoms vibrate with equal amplitudes in the optical as well as acoustical mode
- d. Both types of atoms vibrate, but with unequal, non-zero amplitudes in the optical as well as acoustical mode

5- Consider the energy  $E$  in the first Brillouin zone as a function of the magnitude of the wave vector  $k$  for a crystal of lattice constant  $a$ . Then

- a. The slope of  $E$  versus  $k$  is proportional to the group velocity
- b. The slope of  $E$  versus  $k$  has its maximum value at  $|k| = \frac{\pi}{a}$
- c. The plot of  $E$  versus  $k$  will be parabolic in the interval  $-\frac{\pi}{a} < |k| < \frac{\pi}{a}$
- d. The slope of  $E$  versus  $k$  is non-zero for all  $k$  the interval  $-\frac{\pi}{a} < k < \frac{\pi}{a}$

6- For a free electron gas in two dimensions, the variation of the density of states,  $N(E)$  as a function of energy  $E$ , is best represented by



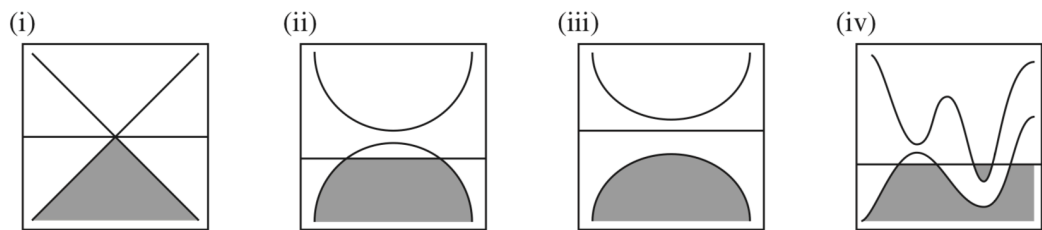
7- For an electron moving through a one-dimensional periodic lattice of periodicity  $a$ , which of the following corresponds to an energy eigenfunction consistent with Bloch's theorem?

- a.  $\psi(x) = A \exp\left(i \left[ \frac{\pi x}{a} + \cos\left(\frac{\pi x}{2a}\right) \right]\right)$
- b.  $\psi(x) = A \exp\left(i \left[ \frac{\pi x}{a} + \cos\left(\frac{2\pi x}{a}\right) \right]\right)$
- c.  $\psi(x) = A \exp\left(i \left[ \frac{2\pi x}{a} + i \cosh\left(\frac{2\pi x}{a}\right) \right]\right)$
- d.  $\psi(x) = A \exp\left(i \left[ \frac{\pi x}{a} + i \left| \frac{\pi x}{2a} \right| \right]\right)$

8- The Bloch theorem states that, within a crystal, the wave function  $\psi(\vec{r})$ , of an electron has the form

- $\psi(\vec{r}) = u(\vec{r})e^{i\vec{k}\vec{r}}$ , where  $u(\vec{r})$  is an arbitrary function and  $\vec{k}$  is an arbitrary vector
- $\psi(\vec{r}) = u(\vec{r})e^{i\vec{k}\vec{r}}$ , where  $u(\vec{r})$  is an arbitrary function and  $\vec{G}$  is a reciprocal lattice vector
- $\psi(\vec{r}) = u(\vec{r})e^{i\vec{k}\vec{r}}$ , where  $u(\vec{r}) = u(\vec{r} + \vec{A})$ ,  $\vec{A}$  is a lattice vector and  $\vec{G}$  is a reciprocal lattice vector
- $\psi(\vec{r}) = u(\vec{r})e^{i\vec{k}\vec{r}}$ , where  $u(\vec{r}) = u(\vec{r} + \vec{A})$ ,  $\vec{A}$  is a lattice vector and  $\vec{k}$  is an arbitrary vector

9- The band structures (energy versus wavevector) shown below are all drawn on the same scale. The Fermi energy is indicated with a horizontal line, and the filled states are shaded.



Which of these statements is incorrect?

- In the case of (iv), there are two contributions of opposite sign to the Hall current
- (ii), (iii), and (iv) show a gap in the electronic density of states
- (ii) and (iv) are likely to be the best conductors
- (i) and (iii) have a vanishing electronic density of states at the Fermi energy.

10- Which of the following is true about the density of states in  $k$ -space? (rem)

- It depends on the dimensionality of the semiconductor.
- States are spaced uniformly in  $k$ -space.
- It is independent of the semiconductor's band structure.
- All of the above.

11- Bloch oscillations—the back-and-forth motion of particles in a periodic potential subject to a constant force—are not typically observed for metallic electrons in real materials. Why?

- The electronic dispersion in a crystal is very nearly parabolic.
- An applied electric field couples equally and oppositely to electrons and holes.
- Scattering times for electrons (due to lattice defects) are too short.

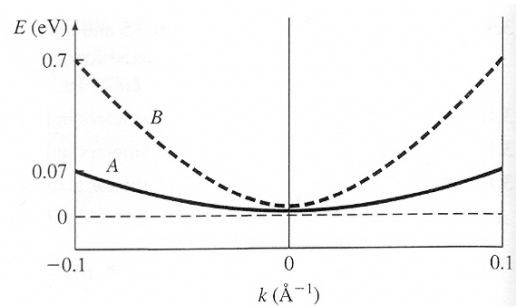
- 12- In a two dimensional band structure energy is given by  $E(k_x, k_y) = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*}$ . What is the shape of the constant energy “surface.” ?
- a line
  - a circle
  - an ellipse
  - a sphere
  - an ellipsoid
- 13- If the number density of free electrons in three dimensions is increased eight times, its Fermi temperature will
- increase by a factor of 4
  - decrease by a factor of 4
  - increase by a factor of 8
  - decrease by a factor of 8
- 14- Which band structure below best describes graphene? (ana)
- $E = E_c + \frac{\hbar^2 K^2}{2m_n^*}$
  - $E = E_v - \frac{\hbar^2 K^2}{2m_p^*}$
  - $E = \pm \hbar v_f k$
  - $E = \pm \hbar v_f k^2$

### Examples for Summative assessment

- Given that the fermi energy of gold is 5.54 eV, the number density of electron is ..... $\times 10^{28}$  per  $m^{-3}$
- In the class, to obtain the expression for Fermi function, we created an N electron state from an N+1 electron state. Also, we assumed that  $f_i N = f_i N+1$  as N is very large. If you are asked to create an N-1 electron state from an N electron state, suggest the necessary changes you will make in the relevant equations (given in the book/note) in order to get the accurate expression for the Fermi function.
- (a) Write the full Hamiltonian that describes the electron motion in solids. Explain each term of the Hamiltonian. What conditions will you apply to accept the free electron theory?  
 (b) If you recall our discussion in the class, we applied certain boundary condition to solve the Hamiltonian.

- (i) Justify the boundary condition.
- (ii) Sketch to compare the eigenstates of a metallic bulk and the corresponding thin film.

4- Figure shows the parabolic  $E$  versus  $k$  relationship in the conduction band for an electron in two particular semiconductor materials. Determine the effective mass (in units of the free electron mass  $m$ ) of the two electrons



5- Show that when the lattice constant,  $a$ , is sufficiently small, the numerical dispersion reduces to the parabolic dispersion:

$$E(k) - U_0 = \frac{\hbar^2 k^2}{2m^*}$$

- 6- Derive an expression for the density-of-states in energy for a 1D semiconductor for states near the centre of the band at  $k_x = 0$ . Assume a valley degeneracy of  $g_v$ .
  - a) Assume a parabolic dispersion near  $k_x = 0$ .
  - b) Assume a linear dispersion near  $k_x = 0$ .

**Resource:** <https://ece.colorado.edu/~bart/book/book/title.htm>

**CO 6:** Students will be able to **analyze** the lattice vibration phenomenon (thermal properties) in the solids

S.No.	LO-6	Pedagogical Decision	Brief Description	Sample Technology
6	<b>Solve Correlate Justify</b>	Jigsaw	Jigsaw is cooperative learning technique. <b>Teacher:</b> will make main groups with 5/6 students in each; one subtopic will be providing to each student in all groups <b>Students:</b> students with same subtopic will work in group and teach subtopic to their peers in main group after preparing  Teacher will provide problems to students	Computer for literature survey, Formative assessment feedback, sharing information with class



		Problem solving by Think-Pair-Share	Student will first think how to proceed individually and then will discuss in group and solve the problem Process will be followed up by teacher	
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### Assessment Plan for LO-6

Type of assessment	Frequency of assessment	Delivery from the learner	Data collection	Learning Verification	Decision making
<b>Formative</b>	After achieving LO	1- Students' generated question 2- peer evaluation 3- MCQ	Softcopy /hard copy	Written Feedback on worksheet on group sheet (computer) Verbal feedback	
<b>Summative</b>	End session (may contain previous LOs)	Test paper	Hard copy	Evaluate and grading of the hard copy; Weightage: 50%	

#### Preparation for jigsaw for teacher

1. Choose a suitable topic and write 5-6 subtopics for the same
2. Divide your class in groups (of students). Each should have 5-6 members (depending on subtopics)
3. Give one subtopic to each group member.
4. The member of each group, having same subtopic can form group and work together on the topic
5. After achieving command on the subtopic, the group members will go to their parent group and teach their respective subtopic to other group members.

#### Teacher's Role:

- 1- Selection of topic and subtopics
- 2- Assign the subtopic to student (teacher can do background work for finding suitable student for a subtopic)
- 3- Help the student in making work plan, progressing forward and giving feedback
- 4- Assessment plan

#### Student's Role

- 1- Students will work in group (Topic group) to learn their subtopic
- 2- They will teach their subtopic to the members of their parent group

Subtopic: (representative/examples)

- Lattice Vibrations of 1D crystals
- Monoatomic chain
- Diatomic chain
- Periodic boundary conditions
- Lattice Vibrations of 3D crystals
- Born–von Karman boundary condition

**Assessment by student's generated questions:**

- 1- Teacher will provide stems for questions generation
- 2- Student will generate the question within parent group (jigsaw group)  
(different type question MCQ, True/false, short questions)
- 3- Along with teacher, there will be peer assessment with rubric

*Assessment Rubric and peer evaluation given in appendix*

**Example questions for formative assessment**

- 1- Suppose the frequency of phonons in a one-dimensional chain of atoms is proportional to the wave vector. If  $n$  is the number density of atoms and  $c$  is the speed of the phonons, then the Debye frequency is
  - a.  $2\pi cn$
  - b.  $\sqrt{2} \pi cn$
  - c.  $\sqrt{3} \pi cn$
  - d.  $\frac{\pi cn}{2}$
- 2- Consider a metal which exactly obeys the Sommerfeld model ~~exactly~~. If  $E_f$  is the fermi energy of the metal at  $T=0$  K and  $R_H$  is its Hall coefficient, which of the following statements is correct
  - a.  $R_H \propto E_f^{3/2}$
  - b.  $R_H \propto E_f^{2/3}$
  - c.  $R_H \propto E_f^{-3/2}$
  - d.  $R_H$  is independent of  $E_f$
- 3- A linear diatomic lattice of lattice constant  $a$  with masses  $M$  and  $m$  ( $M > m$ ) are coupled by a force constant  $C$ . the dispersion relation is given by

$$\omega^2 = C \left( \frac{M+m}{Mm} \right) \pm \left[ C^2 \left( \frac{M+m^2}{Mm} \right) - \frac{4C^2}{Mm} \sin^2 \frac{Ka}{2} \right]^{1/2}$$

which one of the following statement is correct?

- a. The atom vibrating in transverse mode correspond to the optical branch
- b. The maximum frequency of the acoustic branch depends on the mass of the lighter atom  $m$
- c. The dispersion of the frequency in the optical branch is smaller than in the acoustic branch
- d. No normal modes exist in the acoustic branch for any frequency greater than the maximum frequency at  $k = \pi/a$

4- In a cubic crystal, atom of mass  $M_1$  lie on one set of planes and atoms of the mass  $M_2$  lie on planes interleaved between those of the first set. If  $C$  is the force constant between nearest neighbors planes, the frequency of the lattice vibrations for the optical phonon branch with wave vector  $k=0$  is

- a.  $\sqrt{2C \left( \frac{1}{M_1} + \frac{1}{M_2} \right)}$
- b.  $\sqrt{C \left( \frac{1}{2M_1} + \frac{1}{M_2} \right)}$
- c.  $\sqrt{C \left( \frac{1}{M_1} + \frac{1}{2M_2} \right)}$
- d. 0

5- The dispersion relation for 1 D monoatomic crystal with lattice spacing  $a$  which interact via nearest neighbor harmonic potential is given by

$$\omega = \left| \sin \frac{ka}{2} \right| \text{ where } a \text{ is constant of appropriate unit (common data for 2 and 3 )}$$

The group velocity at boundary of the Brillouin zone is

- a. Zero
- b. 1
- c.  $\sqrt{\frac{Aa^2}{2}}$
- d.  $\frac{1}{2} \sqrt{\frac{Aa^2}{2}}$
- e.  $\tau < \tau_m < \tau_E$ .
- f.  $\tau \approx \tau_m \approx \tau_E$ .

6- Why is it that optical phonon scattering requires the initial kinetic energy to be greater than the optical phonon energy?

- a. So that phonon absorption does not occur.
- b. So that that phonon absorption is greater than phonon emission.
- c. So that there are final states to scatter to.
- d. So that that stimulated phonon emission equals spontaneous phonon emission.

- e. None of the above.

### Example questions for summative exam

- 1- The dispersion relation for phonons in a one dimensional monoatomic Bravais lattice with lattice spacing  $a$  and consisting of ions of masses  $M$  is given by

$$\omega(k) = \sqrt{\frac{2c}{M} [1 - \cos(ka)]}, \text{ where } \omega \text{ is the frequency of oscillation, } k \text{ is the wavevector and } c \text{ is the spring constant. For the long wavelength mode}$$

( $\lambda \gg a$ ), find the ratio of phase and group velocities.

- 2- The dispersion relation of electrons in a 3 dimensional lattice in the tight binding approximation is given by

$$\epsilon_k = \alpha \cos k_x a + \beta \cos k_y a + \gamma \cos k_z a \text{ Where } a \text{ is lattice constant and } \alpha, \beta, \gamma \text{ are the constants with the dimension of energy. Find out the effective mass tensor at the corner of the first Brillouin zone } \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right).$$

- 3- Consider a metallic nanowire. Apply the Sommerfeld theory to
- Deduce the electron specific heat capacity and bulk modulus of the wire
  - Obtain an expression for temperature dependent thermo power

### Note:

- All the sessions can be accomplished by lecture and any other pedagogy
- All the examples have taken from GATE, UGC-NET previous years question paper, IIT Madras exam questions and NPTEL

### Reference

- <https://ocw.mit.edu/courses/physics/8-231-physics-of-solids-i-fall-2006/assignments/>
- <https://sites.ualberta.ca/~kbeach/phys308/docs/Final.pdf>
- [https://nptel.ac.in/courses/112108150/pdf/MCQs/MCQ\\_m2.pdf](https://nptel.ac.in/courses/112108150/pdf/MCQs/MCQ_m2.pdf)
- <https://nanohub.org/courses/ece656/offerings>
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