NTNU – Trondheim
Norwegian University of
Science and Technology

Department of physics

Examination paper for TFY4220 Solid State Physics

Academic contact during examination: Randi Holmestad
Phone: 48170066

Examination date: 16. May 2014
Examination time (from-to): 09.00 to 13.00
Permitted examination support material:
C (simple calculator, English dictionary, Rottmann formulas book).
Other information:

Language: English (page 2-5) / Bokmål (page 6-9) / Nynorsk (page 10-13)
Number of pages: 13 (including front page)
Number of pages enclosed: 0

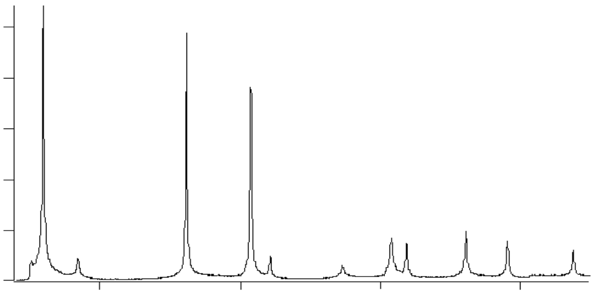
Checked by:

Date Signature

Problem 1 (15%) Introductory questions

Keep your answers to this problem brief!

a) You have done an X-ray scattering experiment, and the result is like the figure. Label the axes, and discuss factors which determine the width and the height of the measured diffraction peaks.



X-ray scattering results

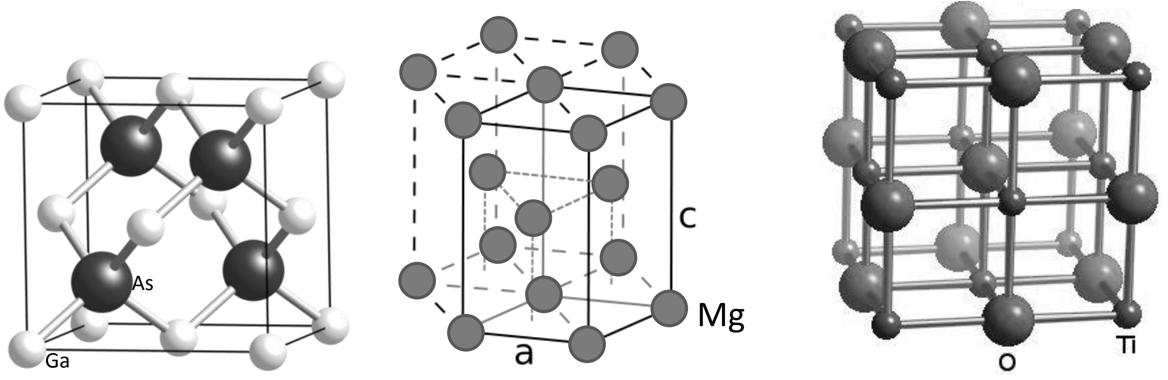
b) What is meant by the first Brillouin zone? Also explain higher zones, and when the concept of the Brillouin zones is useful.

c) Sketch a typical electron band structure of a pure semiconductor. Describe what happens to the band structure if impurities (such as donors or acceptors) of very low concentration are added to the specimen. Explain the difference between a direct and indirect bandgap semiconductor.

d) What are Bloch functions? Explain why these are important in solid state physics.

Problem 2 (30%) Structure and Diffraction

a)



I- GaAs *II – Mg* *III - TiO*

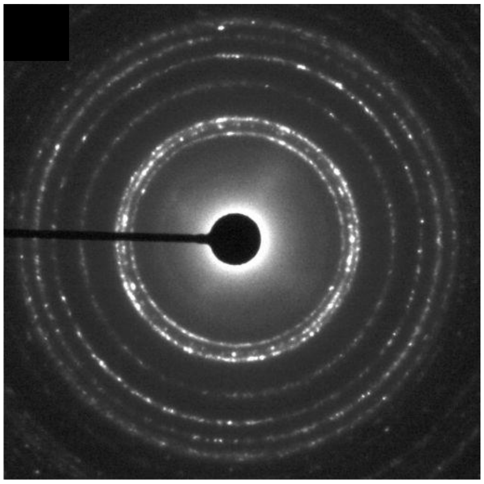
The figures above show the structure of three different materials. *I* is gallium arsenide, *II* is magnesium and *III* is titanium oxide. Specify the Bravais lattice and the basis in each case (you can draw the figure and indicate the atoms belonging to the basis or write down the coordinates). For each case, how many atoms does the basis contain?

b) The packing fraction (PF) is the fraction of the volume in a crystal structure that is occupied by atoms. (By convention, we assume that atoms are hard spheres, and the radius of the spheres is taken to be the maximal value such that the atoms just not overlap.) Calculate the PF of structure *I*, assuming that the two types of atoms are the same. Show that an axial ratio of $c/a = (8/3)^{1/2}$ in structure *II* above optimizes the PF. For this optimised ratio, calculate the PF of structure *II*. What is this structure called? Compare the two PFs and comment.

c) Determine the structure factor and find the extinction rules for TiO (structure *III* above). The structure factor is given by $S_G = F_{hkl} = \sum_j f_j \exp\left(-i\vec{G}_{hkl} \cdot \vec{r}_j\right)$.

Assume that f_j is close to the atom number of *j*. Oxygen is atom number 8 and titanium is atom number 22 in the periodic system. Write down the three lowest reflections for TiO, and sort them according to the intensity in the reflections. Explain your answer.

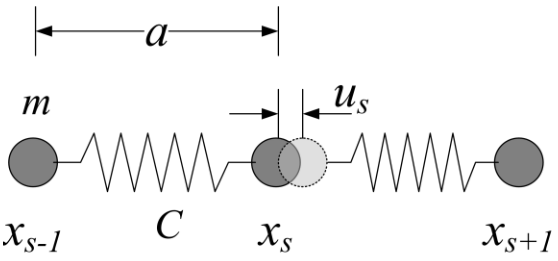
d)



The figure shows a ‘selected area’ diffraction pattern taken in a transmission electron microscope (TEM). (The needle set in from the left is put there to avoid saturation of the camera and has nothing to say for this exercise.) What conclusions can you draw about the material from this image? (You should not index this pattern!)

TEM diffraction pattern

Problem 3 (30%) Phonons



A linear chain of atoms.

a) We have a linear one-dimensional chain of identical atoms with mass *m* as shown in the figure above. Assume interactions only between nearest neighbors, where the harmonic spring stiffness (spring constant) is given by *C*. Set up the motion equation, assume plane wave solutions and show that the dispersion relation is : $\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\tfrac{1}{2}Ka\right)\right|$.

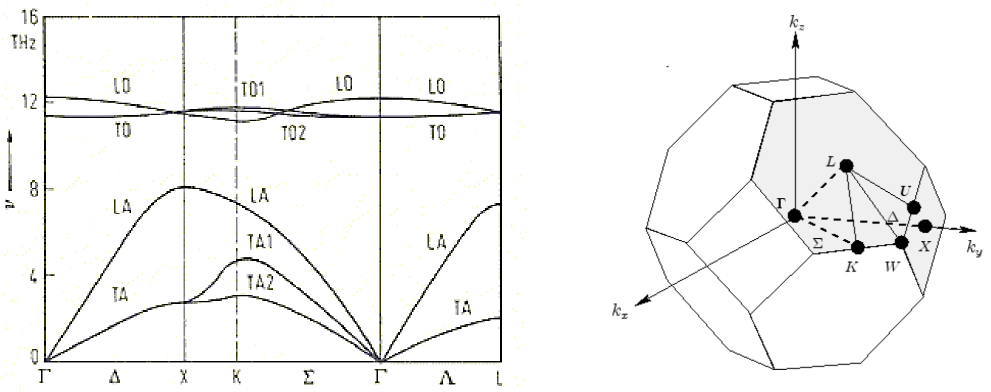
Sketch the phonon dispersion relation. Explain why we can limit the dispersion curves to the first Brillouin zone (1BZ).

b) Assume that the total length of the atomic chain is $L = Na$ (*N*= number of atoms) and use periodic boundary conditions to find that the distance between the permitted states in the reciprocal space is $\Delta K = \frac{2\pi}{L}$. Use this to find the density of states as a function of frequency.

c) Explain what the Debye approximation is and when it is valid. Show that the density of states with the Debye approximation can be written as

$$D(\omega) = \frac{L}{\pi a}\sqrt{\frac{m}{C}} = \frac{L}{\pi v_g}.$$ Define all symbols used.

d) Below is the phonon dispersion relation for a crystal with an fcc structure. How many atoms are there in the primitive unit cell? Explain. How are such curves established (theoretically and experimentally)? Answer short!



Phonon dispersion relation

Problem 4 (25%) Free-electron model and semiconductors

The energy-wave vector dispersion relation for free electrons is $E = \hbar^2 k^2 / 2m$

a) Explain the term Fermi energy E_F , and the difference between the Fermi energy and the chemical potential (or Fermi level) μ. Find the expression for the density of states $D(E)$ for a free electron gas (in three dimensions) under periodic boundary conditions.

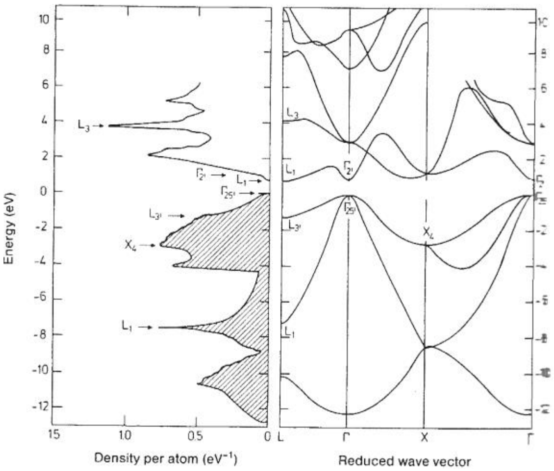
b) The probability that an orbital at energy E is occupied in an ideal Fermi gas in thermal equilibrium at temperature T is given by the Fermi-Dirac distribution

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}.$$

Sketch $D(E) \cdot f(E)$ versus E for the two cases $T = 0$ and $T > 0$.

When the system is heated from absolute zero to T (where $0 < k_B T \ll \mu$), which electrons can be excited thermally? What is the magnitude of the energy gain for such excited electrons? Estimate the number of electrons that would be thermally excited and the total electronic thermal kinetic energy for $T > 0$. Describe how the electron heat capacity behaves at low temperatures.

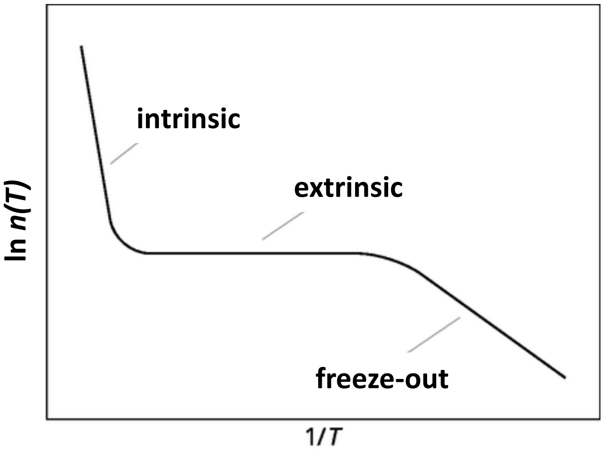
c)



The figure shows the total density of states and the electron dispersion relation in a few k directions of a given crystal. What can you say about this material?

Density of states and electron dispersion relation

d) For an n-type semiconductor, the logarithm of concentration of the major carrier as a function of inverse temperature is plotted in the figure. Explain shortly why $\ln n(T)$ can be characterized by three regions and the physics behind this curve. Give an estimate of the typical temperature range of each region.

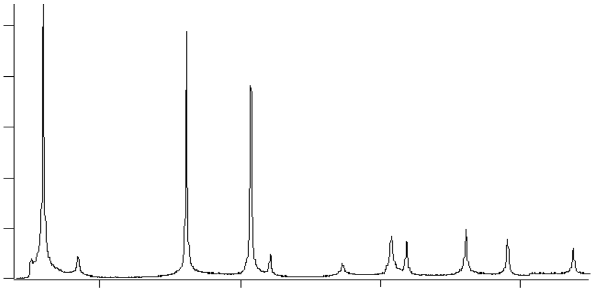


BOKMÅL:

Oppgave 1 (15%) Introduksjonsspørsmål

Svar kort på disse spørsmålene!

a) Du har gjort et Røntgenspredningseksperiment, og resultatet er som figuren. Angi aksene, og diskuter faktorer som bestemmer bredden og høyden av de målte diffraksjonstoppene.



Røntgenspredningsresultat

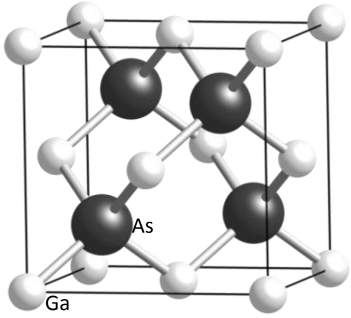
b) Hva menes med første Brillouinsone? Forklare også høyere soner, og når konseptet med Brillouinsoner er nyttig.

c) Tegn en typisk elektronbåndstruktur i en ren halvleder. Beskriv hva som skjer med båndstrukturen hvis vi tilsetter forurensninger (som donorer eller akseptorer) i svært lav konsentrasjon. Forklar forskjellen mellom en direkte og indirekte båndgap i halvledere.

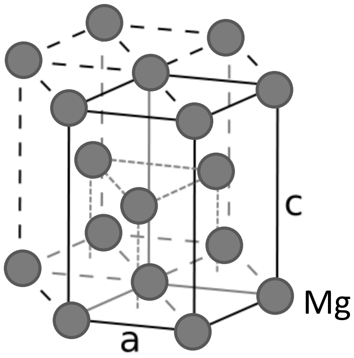
d) Hva er Bloch funksjoner? Forklar hvorfor de er viktige i faststoff-fysikken.

Oppgave 2 (30%) Struktur og diffraksjon

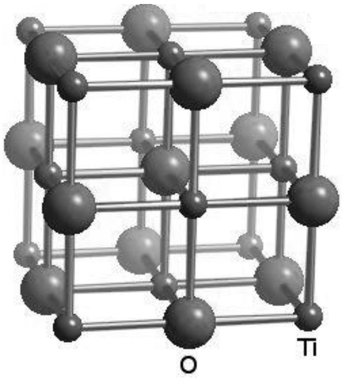
a)



I- GaAs



II – Mg



III - TiO

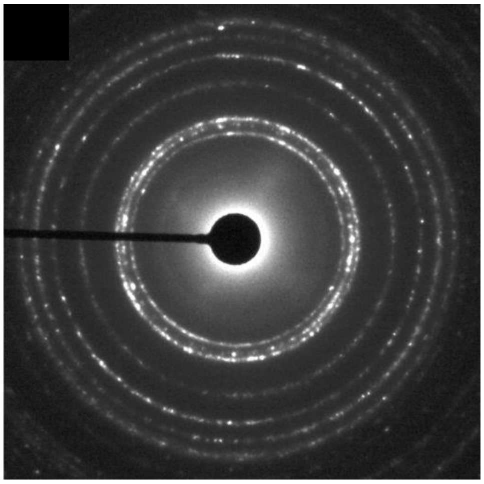
Figurene ovenfor viser strukturen av tre forskjellige materialer. *I* er galliumarsenid, *II* er magnesium og *III* er titanoksid. Spesifiser Bravaisgitteret og basisen i hvert enkelt tilfelle (du kan tegne figuren og vise atomene som tilhører basis eller skrive ned koordinater i enhetscella). For hvert tilfelle, hvor mange atomer er det i basis?

b) Pakkefraksjonen (PF) er den brøkdelen av volumet i en krystallstruktur som er okkupert av atomer. (Vi antar atomene som harde kuler, og radiusen på kulene settes til den maksimalt mulige verdien slik at atomene ikke overlapper hverandre.) Beregn PF av struktur *I*, forutsatt at de to typene av atomer er de samme. Vis at akseforholdet $c/a = (8/3)^{1/2}$ i struktur *II* ovenfor optimaliserer PF. Beregn PF av struktur *II* med dette optimale forholdet. Hva kalles denne strukturen? Sammenlign de to PFene og kommenter.

c) Bestem strukturfaktoren og finn utslokningsregler for TiO (struktur *III* ovenfor). Strukturfaktoren er gitt ved $S_G = F_{hkl} = \sum_j f_j \exp\left(-i\vec{G}_{hkl} \cdot \vec{r}_j\right)$.

Anta at f_j er tilnærmet lik atomnummeret j. Oksygen har atomnummer 8 og titan har atomnummer 22 i det periodiske system. Skriv opp de tre laveste refleksene til TiO som vi får ved et diffraksjonseksperiment og angi rekkefølge av styrken (intensiteten) i de tre refleksene. Begrunn svaret.

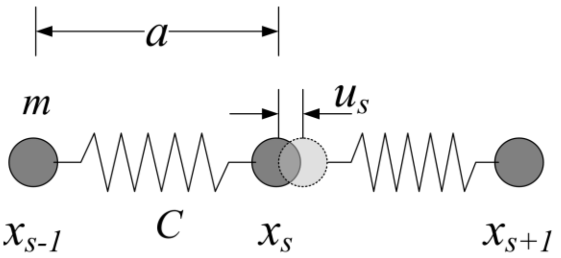
d)



Figuren viser et ‘selected area’ diffraksjonsbilde tatt i transmisjonselektronmikroskopet (TEM). (Nålen inn fra venstre er satt inn for at kameraet ikke skal bli mettet i midten og har ingenting å si for oppgaven.) Hvilke konklusjoner kan du trekke om prøven og materialet ditt ut ifra dette bildet?

TEM diffraksjonsbilde

Oppgave 3 (30%) Fononer



Lineær kjede av like atomer.

a) Anta en lineær endimensjonal kjede av like atomer med masse *m*. Anta vekselvirkning bare mellom nærmeste naboer hvor den harmoniske fjærstivheten (fjærkonstanten) er gitt ved *C*. Sett opp bevegelsesligningen, anta planbølgeløsning og vis at dispersjonsrelasjonen blir:

$$\omega = \sqrt{\frac{4C}{m}} \left|\sin\left(\tfrac{1}{2} Ka\right)\right| .$$

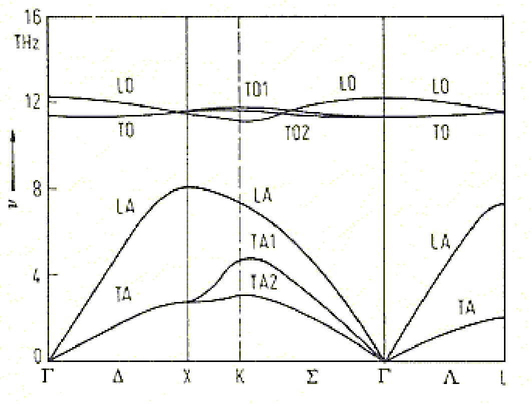
Skisser fonon dispersjonsrelasjonen. Forklar hvorfor dette svingesystemet kan beskrives bare ved hjelp av første Brillouin sone (1BZ).

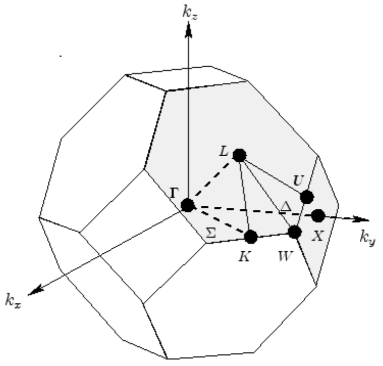
b) Den totale lengden av atomkjeden er $L = Na$. Bruk periodiske grensebetingelser og vis at avstanden mellom tillatte tilstander i det resiproke rom er $\Delta K = \dfrac{2\pi}{L}$. Bruk dette til å finne tilstandstettheten $D(\omega)$ som funksjon av frekvens.

c) Forklar hva Debye-tilnærmingen er og når den er gyldig. Vis at tilstandstettheten med Debye-tilnærmingen kan skrives som

$$D(\omega) = \frac{L}{\pi a}\sqrt{\frac{m}{C}} = \frac{L}{\pi v_g}$$. Definer alle størrelser.

d) Under er en fonon dispersjon for en krystall med en fcc-struktur. Hvor mange atomer er det i den primitive enhetscella? Forklar. Hvordan er slike kurver funnet (teoretisk og eksperimentelt)? Svar kort!





Fonon dispersjonsrelasjonsrelasjon

Oppgave 4 (25%) Frielektronmodell og halvledere

Energi-bølgevektor dispersjonsrelasjonen for frie elektroner er $E = \hbar^2 k^2 / 2m$

a) Forklar begrepet Fermienergi E_F , og forskjellen mellom Fermienergien og det kjemiske potensialet (eller Ferminivået) μ. Finn uttrykket for tetthet av tilstander $D(E)$ for en fri elektrongass (i tre dimensjoner) under periodiske grensebetingelser.

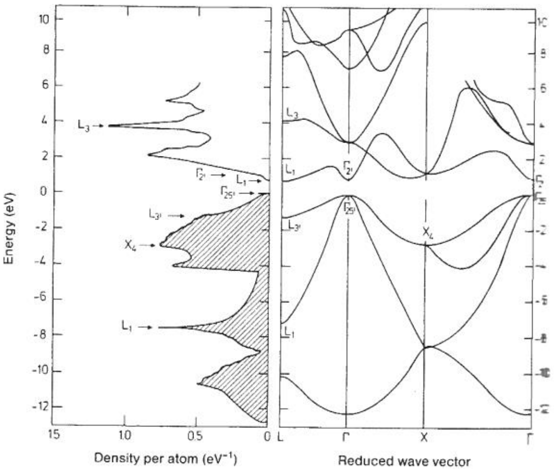
b) Sannsynligheten for at en orbital med energi E er okkupert i en ideell Fermigass i termisk likevekt ved en temperatur T er gitt ved Fermi-Dirac fordelinga

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}.$$

Skisser $D(E) \cdot f(E)$ mot E for de to tilfellene $T = 0$ and $T > 0$.

Når systemet oppvarmes fra absolutt null til T (hvor $0 < k_B T \ll \mu$), hvilke elektroner kan bli termisk eksitert? Hva er størrelsen av den energiøkningen for slike eksiterte elektroner? Estimer antall elektroner som vil være termisk eksiterte og den totale (elektroniske) termiske kinetiske energien. Beskriv hvordan elektron varmekapasiteten er ved lave temperaturer.

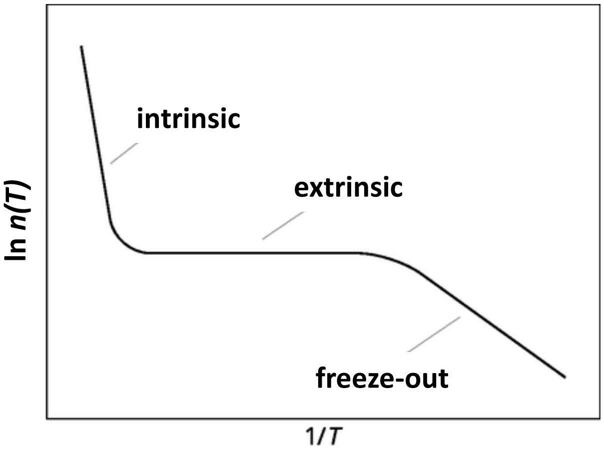
c)



Figuren viser (den totale) tetthet av tilstander og elektrondispersjonreasjonen i noen k retninger i en gitt krystall. Hva kan du si om dette materialet?

Tetthet av tilstander og elektron dispersjonsrelasjon.

d) Figuren viser logaritmen til konsentrasjonen av ladningsbærerne plottet som funksjon av invers temperatur for en n-type halvleder. Forklar kort hvorfor $\ln n(T)$ kan karakteriseres ved tre områder og gi fysikken bak denne kurven. Estimer typisk temperaturintervall for hvert område.



NYNORSK:

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Svar kort på disse spørsmåla!

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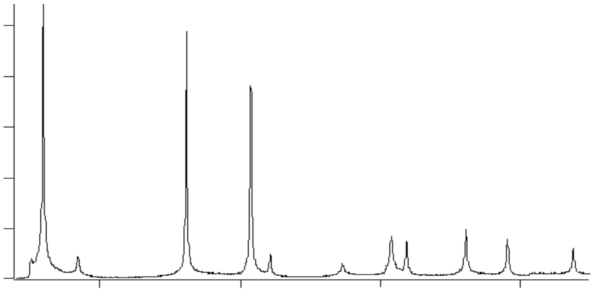


Røntgenspreiingsresultat

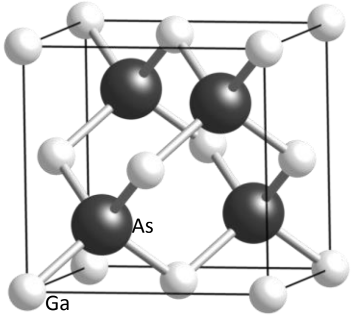
b) Kva meinas med første Brillouinsone? Forklare også høgare soner, og når konseptet med Brillouinsoner er nyttig.

c) Teikn ein typisk elektronbåndstruktur i ein ren halvleder. Forklar kva som skjer med båndstrukturen om vi tilsett forureiningar (som donorer eller akseptorer) i svært lav konsentrasjon. Forklar forskjellen mellom ein direkte og indirekte bandgap i halvleiarar.

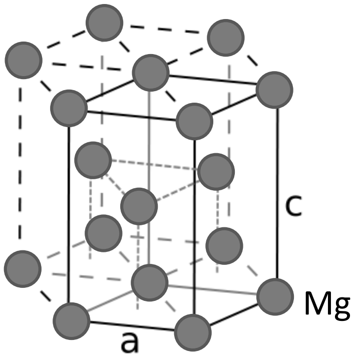
d) Kva er Bloch funksjonar? Forklar kvifor dei er viktige i faststoff-fysikken.

Oppgåve 2 (30%) Struktur og diffraksjon

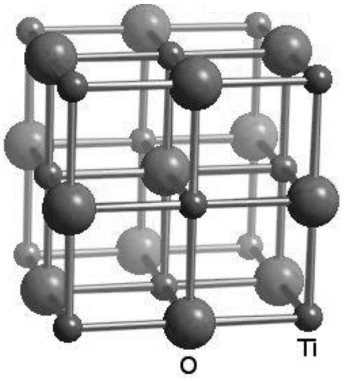
a)



I- GaAs



II – Mg



III - TiO

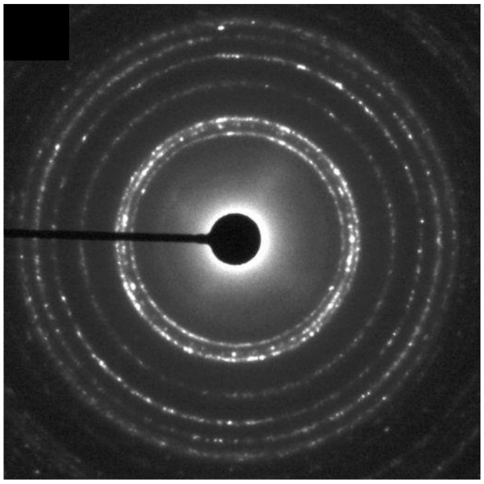
Figurane ovanfor viser strukturen av tre forskjellige materiale. *I* er galliumarsenid, *II* er magnesium og *III* er titanoksid. Spesifiser Bravaisgitteret og basisen i kvart enkelt tilfelle (du kan teikne figuren og vise atomar som høyrar til basis eller skrive ned koordinatar i einhetscella). For kvart tilfelle, kor mange atomar er det i basis?

b) Pakkefraksjonen (PF) er den brøkdelen av volumet i ein krystallstruktur som er okkupert av atomar. (Vi antar atomar som harde kuler, og radiusen på kulene vert sett til den maksimalt mulige verdien slik at atomane ikkje overlappar kvarandre.) Berekn PF av struktur *I*, når ein antar at dei to typane av atomar er dei same. Vis at akseforholdet $c/a = (8/3)^{1/2}$ i struktur *II* ovanfor optimaliserer PF. Berekn PF av struktur *II* med dette optimale forholdet. Kva kallas denne strukturen? Samanlikn de to PFene og kommenter.

e) Finn eit utrykk for strukturfaktoren og finn utslokningsreglar for TiO (struktur *III* ovanfor). Strukturfaktoren er gitt ved $S_G = F_{hkl} = \sum_j f_j \exp\left(-i\vec{G}_{hkl} \cdot \vec{r}_j\right)$.

Anta at f_j er tilnærma lik atomnummeret j. Oksygen har atomnummer 8 og titan har atomnummer 22 i det periodiske system. Skriv opp dei tre lågaste refleksane til TiO som vi får ved et diffraksjonseksperiment og angi rekkefølgje av styrken (intensiteten) i de tre refleksane. Gje grunn for svaret.

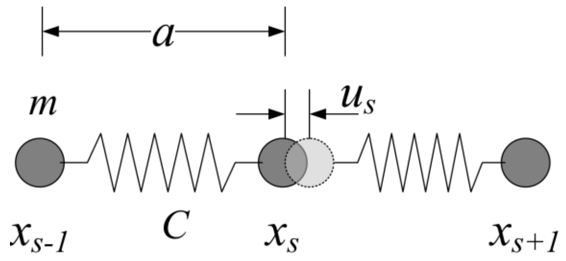
d)



Figuren viser et ‘selected area’ diffraksjonsbilde tatt i transmisjonselektronmikroskopet (TEM). (Nåla inn frå venstre er satt inn for at kameraet ikkje skal bli metta i midten og har ingenting å si for oppgåva.) Kva slags konklusjonar kan du trekke om prøven og materialet ditt ut ifrå dette bildet?

TEM diffraksjonsbilde

Oppgåve 3 (30%) Fononer



Lineær kjede av like atomar.

e) Anta ei lineær eindimensjonal kjede av like atomar med masse *m*. Anta vekselverking bare mellom nærmaste nabo kor den harmoniske fjærstivheten (fjærkonstanten) er gitt ved *C*. Sett opp bevegelseslikninga, anta planbølgjeløysning og vis at dispersjonsrelasjonen blir:

$$\omega = \sqrt{\frac{4C}{m}} \left| \sin\left(\tfrac{1}{2} Ka\right) \right| .$$

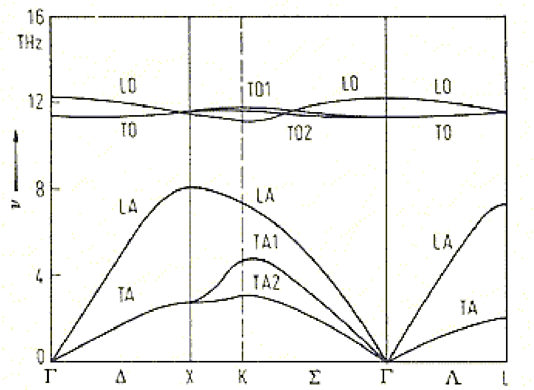
Skisser fonon dispersjonsrelasjonen. Forklar kvifor dette svingesystemet kan synast berre ved hjelp av første Brillouin sone (1BZ).

f) Den totale lengda av atomkjeda er $L = Na$. Bruk periodiske grensebetingelser og vis at avstanden mellom tillate tilstandar i det resiproke rom er $\Delta K = \frac{2\pi}{L}$. Bruk dette til å finne tilstandstettheten $D(\omega)$ som funksjon av frekvens.

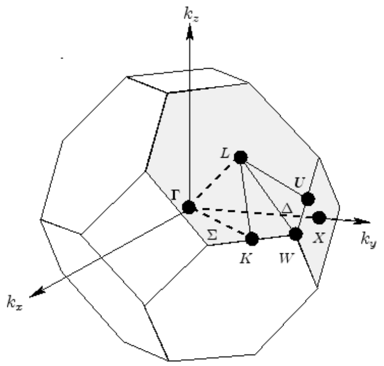
g) Forklar kva Debye-tilnærminga er og når den er gyldig. Vis at tilstandstettheten med Debye-tilnærminga kan skrivas som

$$D(\omega) = \frac{L}{\pi a}\sqrt{\frac{m}{C}} = \frac{L}{\pi v_g}$$. Definer alle storleikar.

h) Under er ein fonon dispersjon for ein krystall med ein fcc-struktur. Kor mange atom er det i den primitive enhetscella? Forklar. Korleis er slike kurver funnet (teoretisk og eksperimentelt)? Svar kort!



Fonon dispersjonsrelasjonsrelasjon



Oppgåve 4 (25%) Frielektronmodell og halvleiarar

Energi-bølgjevektor dispersjonsrelasjonen for frie elektronar er $E = {\hbar^2 k^2}/{2m}$

a) Forklar kva Fermienergi E_F er, og forskjellen mellom Fermienergien og det kjemiske potensialet (eller Ferminivået) μ. Finn uttrykket for tettleik av tilstander $D(E)$ for ein fri elektrongass (i tre dimensjoner) under periodiske grensebetingelser.

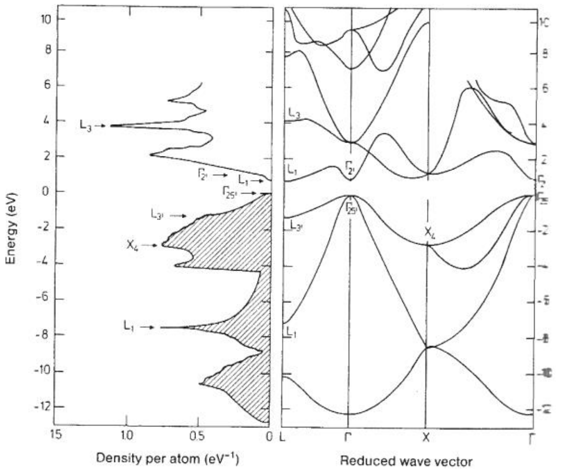
b) Kor sannsynleg det er at ein orbital med energi E er okkupert i ein ideell Fermigass i termisk likevekt ved ein temperatur T er gitt ved Fermi-Dirac fordelinga

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1} .$$

Skisser $D(E) \cdot f(E)$ mot E for de to tilfella $T = 0$ and $T > 0$.

Når systemet vert oppvarma frå absolutt null til T (kor $0 < k_B T \ll \mu$), kva slags elektronar kan bli termisk eksiterte? Kva er storleiken av energiauka for slike eksiterte elektronar? Estimer kor mange elektronar som vil være termisk eksiterte og den totale (elektroniske) termiske kinetiske energien. Beskriv korleis elektron varmekapasiteten er ved lave temperaturar.

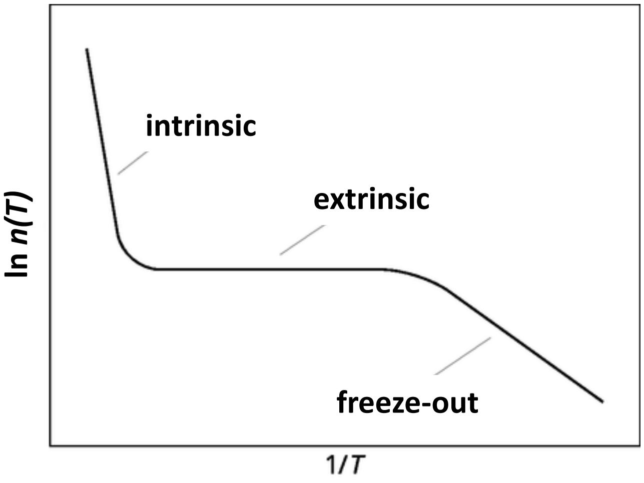
c)



Figuren viser (den totale) tetthet av tilstander og elektrondispersjonreasjonen i noen k retningar i ein gitt krystall. Kva kan du si om dette materialet?

Tetthet av tilstander og elektron dispersjonsrelasjon.

d) Figuren viser logaritmen til konsentrasjonen av ladningsbærerar plotta som funksjon av invers temperatur for ein n-type halvleder. Forklar kort kvifor vi finn tre områder og fysikken bak denne kurva. Estimer eit typisk temperaturintervall for kvart område.

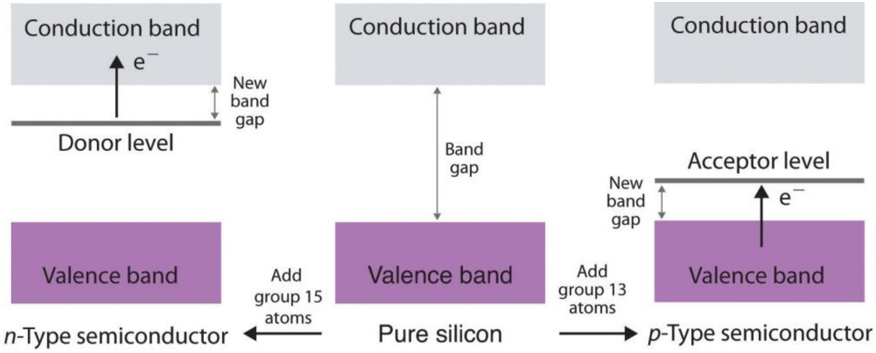


Draft of solution Exam TFY4220, Solid State Physics, 16. May 2014.

Problem 1 (15%) Introductory questions

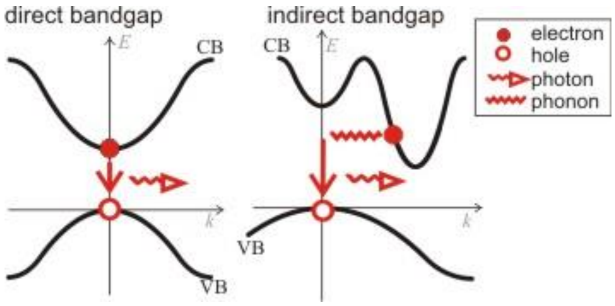
1a) From the lab: Label: Y= Intensity, x=Angle 2theta. Many factors can affect the width and the height of the peaks, but the most important (which should be mentioned) are that width is determined mainly by crystallite size and energy spread in beam in, while height is decided mainly by structure factor

1 b) The first Brillouin zone is a uniquely defined primitive cell in reciprocal space. The boundaries of this cell are given by planes related to points in the reciprocal lattice. It is found by the same method as for the Wigner–Seitz cell in the Bravais lattice. The importance of the Brillouin zone stems from the Bloch wave description of waves in a periodic medium, in which it is found that the solutions can be completely characterized by their behavior in a single Brillouin zone. There are also second, third, etc., Brillouin zones, corresponding to a sequence of disjoint regions (all with the same volume) at increasing distances from the origin, the n-th Brillouin zone consists of the set of points that can be reached from the origin by crossing exactly n − 1 distinct Bragg planes.



1c) Band structure of an intrinsic semiconductor reveals an energy gap between valence band and conduction band. At zero temperature, all states in the valence band are filled and all states in the conduction band are vacant. As temperature is increased, electrons are thermally excited from the valence band to the conduction band where they become mobile. The energy gap is ~1eV. If donors of very low concentration are added to the semiconductor (n-type), the valence electrons of the donors are available for conduction. At zero temperature, the extra valence electron is bounded in donor state, about 10 meV lower than the conduction band edge. As temperature is increased, the electron is excited to the conduction band. Similar for p-type, acceptor states are created above the valence band edge (also about 10 meV), when acceptors are added. At non-zero temperature, acceptor states can capture electrons and leave holes in the valence band. These are then available for conduction

Direct and indirect band gap:



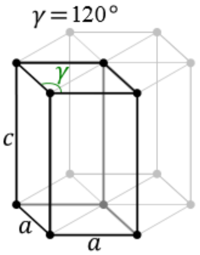
1d) A Bloch function is a function which is a product between a plane wave and a periodic function where r is position, ψ is the Bloch wave, u is a periodic function with the same periodicity as the crystal, k is a real number called the crystal wave vector. $\psi(\mathbf{r}) = \mathrm{e}^{\mathbf{ik}\cdot\mathbf{r}}u(\mathbf{r}),$

This is important in physics because they are the solution of the Schrödinger's equation with periodic potential, and the source of Bloch waves.

Problem 2 (30%) Structure and Diffraction

2a) I GaAs has the diamond structure – which is the fcc (face centered cubic) with two atoms in the basis, here Ga in (000) and As in (¼, ¼, ¼). The fcc Bravais lattice has 4 lattice points in the unit cell – in (000), (½,½, 0), (½,0, ½,), (0, ½,½). For each of these we again have two atoms as a basis, so that there are 8 atoms in the unit cell.

II Mg has a hexagonal Bravais lattice – 2 atoms in basis (0,0,0) and (2/3, 1/3, ½). One lattice point in the hexagonal Bravais lattice. Two atoms in the unit cell.



III TiO has the RockSalt structure – (same as NaCl) which is a fcc structure (4 Bravais lattice points in unit cell) with two atoms in basis – in this case Ti in (000) and O in (½ , ½, ½). Same as for GaAs, but the position of atoms in the basis is different. Fcc Bravais lattice, 2 atoms in basis, 8 atoms in the unit cell.

2b) PF of structure I: Here the largest radius we can have is 1/8 of the diagonal. (√3 a)/8 , and this gives a packing fraction for the diamond structure to be (√3 π)/16≈0,34.

Structure II is hexagonal – for this to be perfect hcp, the c/a has to be $(8/3)^{1/2}$, this was found in the lab – - In the closest packed arrangement of two different layers, each atom in the upper layer sits exactly into the dip among the three touching spheres of the lower layer. Then the height difference between the centers of the spheres of the two layers is √(8/3) r. The lattice parameter In the hexagonal plane has to be 2r to obtain highest packing, and the periodicity along the c direction is twice the repeat distance of the layers, close packing is therefore achieved if c/a= √(8/3)≈1,633. See here for details: http://www.doitpoms.ac.uk/tlplib/slip/ideal_axial_ratio.php. The cell contains two atoms, and the PF is then 0,74. This structure is called hcp, hexagonal closed packed, same value for PF as fcc closed packed. We see that the PF is more than double as high as for structure I.

2c) Two atoms in basis – in this case Ti in (000) and O in (½ , ½, ½). This group repeats in all four Bravais lattice points (0,0,0), (½ ½ 0), (0 ½ ½) and (½ 0 ½) Same as for NaCl,

$S_G = F_{hkl} = \sum_j f_j \exp\left(-i\vec{G}_{hkl}\cdot\vec{r}_j\right)$ We have 8 atoms – Ti in (0,0,0), (½ ½ 0), (0 ½ ½) and (½ 0 ½) and O in (½,½,½), (0 0 ½), (½ 0 0) and (0 ½ 0) This gives

$F_{hkl} = f_{Ti}(1+e^{\pi i(h+k)}+e^{\pi i(k+l)}+e^{\pi i(h+l)}) + f_O(e^{\pi i(h+k+l)}+e^{\pi i(k)}+e^{\pi i(h)}+e^{\pi i(l)})$ Can be simplified to

$$F_{hkl} = (f_{Ti} + f_O e^{\pi i(h+k+l)})(1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)})$$

This gives

$F_{hkl} = 4(f_{Ti} + f_O)$, hkl are all even (strong)

$F_{hkl} = 4(f_{Ti} - f_O)$, for hkl all odd (weak)

$F_{hkl} = 0$ hkl mixed (no reflection)

This gives the three lowest reflections observed 111, 200 and 220 weakest, strongest, strong, respectively. (The statement that *fs is close* to Z is valid only for the forward direction – in general *f* decreases with increasing scattering angle – therefore 200 is stronger than the 220, but since the exercise was slightly misleading, I accept the answer that these two have the same strength..).

2d) Since we see that many reflections in rings, we can conclude that the sample is crystalline, but with many small crystallites. No preferred orientation since the intensity in the ring is even. We have not enough info to know if this is one phase or more, but we could measure the d values and the relation between them. In this case this is from one phase, ZnO, which is hexagonal, but that cannot be known from the info you have.

Problem 3 (30%) Phonons

3 a)

$$\begin{aligned} m\frac{d^2u_s}{dt^2} &= C\left(u_{s+1} - u_s\right) + C\left(u_{s-1} - u_s\right) \\ &= C\left(u_{s+1} + u_{s-1} - 2u_s\right). \end{aligned}$$

The equilibrium atom positions are given by $x_s = s \cdot a$, and the time derivative of the trial solution is $\frac{d}{dt}u_s = -i\omega \cdot u_s$. This gives $-m\omega^2 u_s = C\left[u_s e^{iKa} + u_s e^{iKa} - 2u_s\right]$

The non-trivial solution of this equation gives the dispersion relation

$$-m\omega^2 = C\left(e^{iKa} + e^{-iKa} - 2\right) \quad \Rightarrow \quad \omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\tfrac{1}{2}Ka\right)\right|.$$

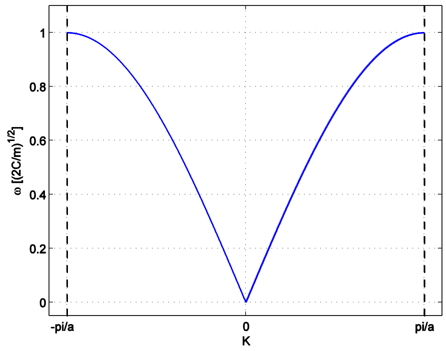


Figure 1: Dispersion relation for monatomic chain

K-values outside the 1BZ represent wavelengths shorter than the periodicity of the lattice. The motion/ position of the atoms can be described by a wave with wavelength inside the 1BZ. This can be shown by adding a general reciprocal lattice vector to a wave outside the 1BZ:

$$u_K = u\exp\left(iKa\right)$$
$$u_{K+G} = u\exp\left(iKa+Ga\right) = u\exp\left(iKa\right)\underbrace{\exp\left(iGa\right)}_{=1}$$
$$u_{K+G} = u_K$$

3b) The function is required to be periodic over a long range: $u\left(na\right)=u\left(na+L\right)$. This gives allowed K-values $K_n = \frac{2\pi}{L}n, \quad n=0,\pm1,\pm2,\ldots, \quad \Delta K = K_n - K_{n-1} = \frac{2\pi}{L}$.

The number of states between K and $K+dK$ is (Multiply by 2 since there is a corresponding negative value) $D\left(K\right)dK = 2\frac{dK}{\Delta K} = \frac{L}{\pi}dK$

As a function of frequency this can be written

$$D\left(\omega\right)d\omega = D\left(K\right)dK \qquad D\left(\omega\right) = D\left(K\right)\frac{dK}{d\omega} = \frac{D\left(K\right)}{d\omega/dK}$$

The group velocity is found as $\frac{d\omega}{dK} = a\sqrt{\frac{C}{m}}\cos\left(\frac{1}{2}Ka\right) = a\sqrt{\frac{C}{m}-\left(\frac{1}{2}\omega\right)^2}$.

(Here we used the dispersion relation to find ω dependency of $\cos\left(\frac{1}{2}Ka\right)$.)

The density of states as a function of frequency is then $D\left(\omega\right) = D\left(K\right)\frac{dK}{d\omega} = \frac{L}{\pi a}\underline{\underline{\frac{1}{\sqrt{\frac{C}{m}-\left(\frac{1}{2}\omega\right)^2}}}}$.

3c) At short wavelengths the dispersion relation is approximately linear to K; $\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{1}{2}Ka\right)\right| \approx \sqrt{\frac{4C}{m}}\frac{1}{2}\left|K\right|a$, which is the case in a classical elastic continuum as the Debye model assumes. Group speed (speed of sound) is $v_g = \omega/K = a\sqrt{C/m}$ - inserting this into $D\left(K\right)$ gives : $D\left(\omega\right) = D\left(K\right)\frac{dK}{d\omega} = \frac{L}{\pi a}\sqrt{\frac{m}{C}} = \frac{L}{\pi v_g}$ as should be shown.

Alternatively the general phonon density of states can be approximated for small K:

$$D(\omega)=\frac{L}{\pi a}\frac{1}{\sqrt{\frac{C}{m}-\left(\frac{1}{2}\omega\right)^2}}=\frac{L}{\pi v_g}\frac{1}{\sqrt{1-\left(\frac{a\omega}{2v_g}\right)^2}}\approx\frac{L}{\pi v_g}\quad\text{since }\ Ka=\frac{\omega a}{v}\ll 1\ .$$

3d) We see there are three optical and three acoustic branches, that means 2 atoms in each primitive cell (3s modes, with s equal atoms per primitive unit cell.)

A direct observation of the dispersion relation for lattice vibrations is not possible because sound waves of sufficiently high frequencies are not available. Methods of observing the dispersion relation of lattice vibrations are inelastic neutron scattering, electron energy loss spectroscopy (EELS) and inelastic atom scattering.

Problem 4 (25%) Free-electron model and semiconductors

4a) The Fermi energy is defined as the energy separating the highest occupied from the lowest unoccupied orbital levels at zero temperature. In a solid with energy band gap, the Fermi energy may locate in the gap. The chemical potential depends on temperature and is often called Fermi level in solid state physics. At zero temperature, the energy $E=\mu$ divides the occupied levels from the empty ones. Therefore, $\mu(T=0)$ is the Fermi energy. See f ex. Kittel Fig 5, chapter 6.

Assume conduction electrons are a free electron gas. No interaction with ions or lattice, or interaction between conduction electrons. Charged particles; follow the Pauli principle $E(k)=\frac{\hbar^2}{2m}k^2$. The Fermi energy is the highest occupied energy, corresponding to the Fermi energy wave vector k_F, corresponding to a sphere in 3D. The number of states inside the sphere with radius k_F is N. The volume in k-space which is occupied by one state is given so that the size of the material is $V=L^3$ in real space; which is $\left(\frac{2\pi}{L^3}\right)$. There is one allowed wave vector for each $\left(\frac{2\pi}{L^3}\right)$ this will then give:

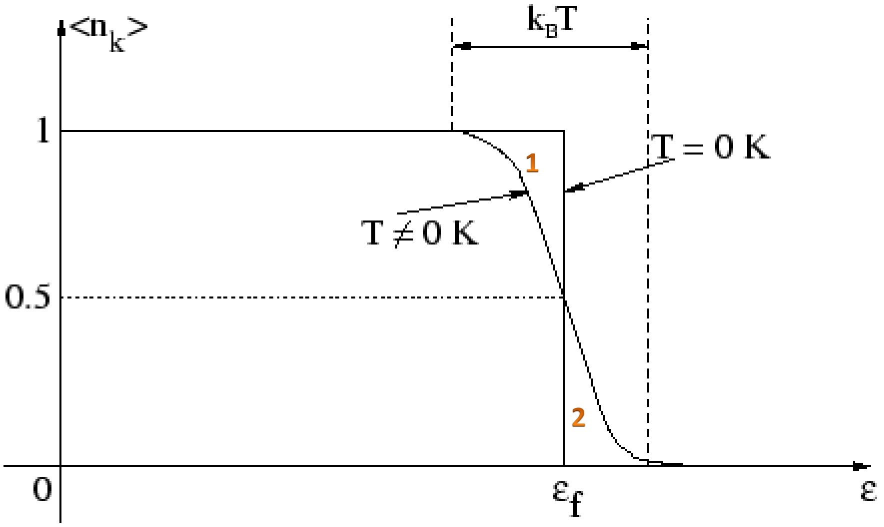
$$N=2\frac{\frac{4}{3}\pi k_F^3}{\left(\frac{2\pi}{L}\right)^3}=\frac{k_F^3V}{3\pi^2}$$ which gives $k_F=\left(\frac{N3\pi^2}{V}\right)^{1/3}$. This gives the Fermi energy

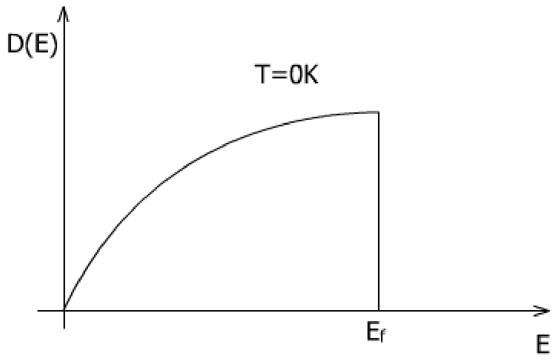
$$E_F=\frac{\hbar^2}{2m}\left(\frac{3N\pi^2}{V}\right)^{2/3}$$. From this expression we can now find the number of states less than E, given by N(E): $E_F=\frac{\hbar^2}{2m}\left(\frac{3N(E)\pi^2}{V}\right)^{2/3}$

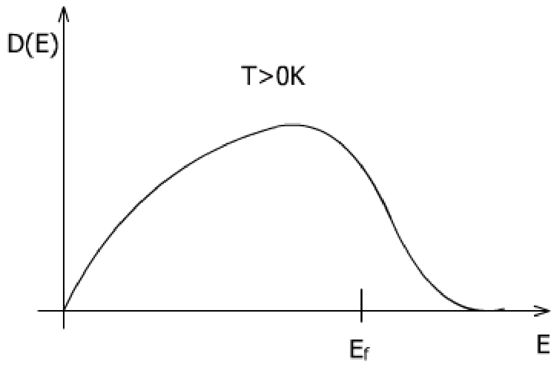
gives $N(E) = \frac{V}{3\pi^2}\left(\frac{E2m}{\hbar^2}\right)^{3/2}$ Then we can find

$$D(E) = \frac{dN}{dE} = \frac{V}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot \frac{3}{2} E^{\frac{1}{2}} = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{\frac{1}{2}}$$

4b) Number of occupied states is given by $D(E)$ multiplied with the probability that the state is occupied, which is given by the Fermi-Dirac distribution $f(E) = \frac{1}{e^{(E-\mu)/k_B T}+1}$. When T>0 we get excitation from area 1 in the figure to area 2, the extension of this areas is typically $k_B T$ as shown in the figure.







At zero temperature, the energy = divides the occupied levels from the empty ones. Therefore, (T =0) is Fermi energy. (see also fig 5 chapter 6 in Kittel or Figure 57 in Hemmer). According to these figure, only those electrons in orbitals within an energy roughly $k_B T$ are excited thermally. The energy gain for such an excited electron is of magnitude $k_B T$. The number of electrons that would be excited is estimated by $D(E_F)\cdot\Delta E \approx \frac{3N}{2E_F}\cdot k_B T$ Therefore, the total electronic thermal kinetic energy is about $U_{el} \approx k_B T\cdot D(E_F)\cdot\Delta E \approx \frac{3NT}{2T_F}\cdot k_B T$. The electronic heat capacity is therefore proportional to T, given by $C_{el} = \frac{\partial U}{\partial T} \approx Nk_B T\frac{3}{T_F}$. (You don't need to write down all these equations, but should then explain this in words..)

4c) This material is a semiconductor, since the $D(E)$ is zero just above the band gap.

4d) Generally we can define three regimes for doped semiconductors. For the n-type we have (p-type case is similar).

1) At low temperatures, in the freeze-out region, not all of the donors are ionised. The slope of a plot of lnn against 1/T will be proportional to the ionisation energy of the donors.

2) At medium temperatures, in the saturation region, all of the donors are ionised but temperatures are still too low to excite many electrons all the way across the band gap. Thus the concentration of electrons in the conduction band is constant with temperature. (It is this region that we have assumed when making the calculation of n above.)

3) At high temperatures, in the intrinsic region, excitation across the band gap dominates the concentration of conduction electrons (there are many more electrons in the valence band than a small donor concentration can provide, as long as they have enough energy to hop across the band gap). In this region, as the name suggests, the equation for n is the same as for the intrinsic case, and the slope of the graph is $-E_g / 2k_B$