Norges teknisk-naturvitenskapelige universitet
Fakultet for naturvitenskap og teknologi
Institutt for fysikk

Bokmål

Faglig kontakt under eksamen:
Navn: Randi Holmestad
Tlf.: 93880 / 48170066

EKSAMEN I FAG TFY4220 Faste stoffers fysikk

Lørdag 9. juni 2012
Tid: 9.00 – 13.00
Norsk bokmål tekst (English text after Norwegian text)

Antall sider: 4 (+ 4 for English text)
Frist for resultat: 30.06.2012

Tillatte hjelpemidler:
Alternativ C (enkel kalkulator, Engelsk ordbok, Rottmann formler).

Vekting på hver oppgave (som brukes ved karaktersetting) er gitt i parentes.

Oppgave 1 (20%) Introduksjonsspørsmål

Svar kort på denne oppgaven!

a) Forklar hva et resiprokt gitter er og hvorfor vi innfører det i faststoff-fysikk. Hva er det matematiske forholdet mellom reelt og resiprokt rom?

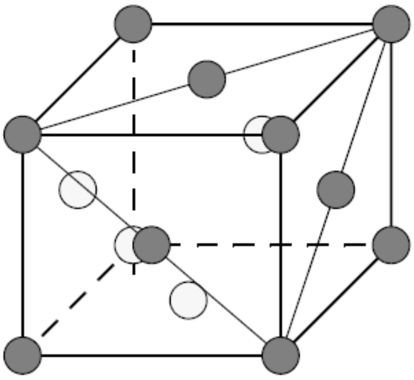
b) Hva menes med varmekapasitet av et materiale? Hva er de viktigste bidragene til varmekapasiteten? Hvilke bidrag dominerer for de ulike typer materialer?

c) Hva mener vi med energibånd? Hva er årsaken til energigap i materialer?

d) Hva menes med Fermi-energi? Når er begrepet "Fermiflate' interessant og hva er det?

Oppgave 2 (25%) Struktur og diffraksjon

a) Figuren viser en konvensjonell fcc (flatesentrert kubisk) enhetscelle med gitterkonstant *a*. Argumenter for at fcc gitteret er et Bravaisgitter. Vis hvordan dette gitteret kan betraktes som et sc (simpelt kubisk) gitter med en fleratomig basis og gi atomposisjonene til alle atomer i basis.
Hvordan kan vi lage en primitiv enhetscelle i fcc gitteret? Tegn den primitive cella og angi vinklene mellom de primitive enhetsvektorene. Hva er volumet av den primitive cella?



b) Hva mener vi med pakkefraksjon? fcc strukturen kan vise det vi kaller 'tetteste kulepakning'. Forklar hva dette er, hvordan det realiseres i fcc og beregn pakkefraksjonen i dette tilfellet.

c) Strukturfaktoren er gitt ved $S_G = F_{hkl} = \sum_j f_j \exp\left(-i\vec{G}_{hkl} \cdot \vec{r}_j\right)$. Forklar alle størrelsene involvert og utled utslokningsreglene for fcc strukturen over.

d) Fluoritt CaF_2 er fcc med Ca^{2+} i hjørner og midt på alle flater og F^- på romdiagonalene i avstand ¼ av diagonalen fra alle hjørnene. Gitterparameteren for CaF_2 er a=5.463 Å ved romtemperatur. Fluor har atomnummer 9 og Kalsium atomnummer 20. Tegn enhetscella og identifiser basis i strukturen. Sett opp S_G for diffraksjon fra CaF_2 uttrykt ved f_{Ca} *og* f_F for de to ione-typene, angi utslokkinger for de laveste *hkl* refleksene.

e) Regn ut diffraksjonsvinklene 2θ for refleksene 400, 331 og 420 for fluoritt når vi har røntgenstråling med bølgelengde λ= 1.542 Å og angi rekkefølge av styrken (intensiteten) i de tre refleksene.

Oppgave 3 (25%) Fononer

Vi tar utgangspunkt i et lineært gitter med to-atomig basis. Gitterkonstanten er a, og avstanden mellom atomene er $a/2$. Atomene har masse M_1 og M_2. Vi skal studere longitudinale bølger og anta vekselvirkning kun mellom nærmeste naboer og at vi har harmoniske krefter. Kraftkonstanten mellom nærmeste naboer er C for den longitudinale svingningen (parallelt med kjeden).

a) Skriv opp bevegelseslikningene. Anta så en bølgeløsning med utsving lik $u_n = u \cdot e^{i(nKa-\omega t)}$ og $v_n = v \cdot e^{i(nKa-\omega t)}$.

Utled dispersjonsrelasjonen:

$$\omega^2 = C\left[(\frac{1}{M_1}+\frac{1}{M_2}) \pm \sqrt{(\frac{1}{M_1}+\frac{1}{M_2})^2 - \frac{4}{M_1 M_2}\cdot\sin^2\frac{Ka}{2}} \right]$$

Vi vil nå studere fononer med lys i det infrarøde (IR) området.

b) Forklar hvorfor vi med IR absorpsjon i krystaller generelt bare kan studere den sentrale delen av Brillouinsonen. Finn gruppehastigheten ($v = \partial\omega / \partial K$) for akustisk og optisk grein i grensen $K \to 0$ for det lineære gitteret over.

c) Bruk forholdet mellom u og v til å si noe om forskjellen på optiske og akustiske fononmoder. Hvordan er sammenhengen mellom naboatomene? Forklar forskjellen på transversale og longitudinale moder. For transversale moder vil kraftkonstanten *C* generelt være svakere enn for longitudinale moder. Vil lydhastigheten for longitudinale moder være større eller mindre enn for transversale moder? Hva er typisk størrelsesorden på lydhastigheter i faste stoffer?

d) I realistiske systemer kan det være svært vanskelig å beregne dispersjonsrelasjonen, og Debye-approksimasjonen er mye brukt. I Debye-approksimasjonen brukes dispersjonsrelasjonen $\omega = vK$ hvor *v* er lydhastigheten. Lag en skisse og forklar hva som ligger i denne approksimasjonen. For å beregne termodynamiske størrelser trenger vi tetthet av tilstander. Forklar hvordan du ville gå fram for å bestemme tetthet av fonontilstander $D(\omega)$ og finn $D(\omega)$ i Debye-approximasjonen i det en-dimensjonale tilfellet. Til tross for at det er en grov approksimasjon gir Debye-modellen riktig temperaturforløp i uttrykket for varmekapasiteten. Forklar hvorfor.

Oppgave 4 (30%) Fri-elektronmodell, energibånd og halvledere

a) Gi en kort og kvalitativ beskrivelse av fri-elektronmodellen. Vi skal nå studere *N* frie elektroner i en kube med sidekant *L*. Anta periodiske grensebetingelser og at temperaturen er *T*=0. Bestem tettheten av *k*-verdier i *k*-rommet. Definer Fermi-energien E_F og vis at utrykket for Fermi-bølgevektoren kan skrives $k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}}$ med volum $V = L^3$

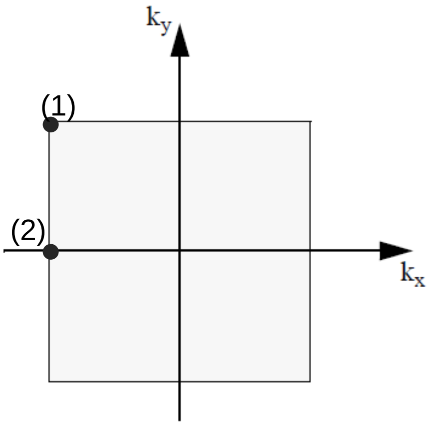
Vis at tetthet av tilstander (antall tilstander per energienhet) *D(E)* i 3 dimensjoner er gitt ved

$$D(E) = CE^{1/2}$$

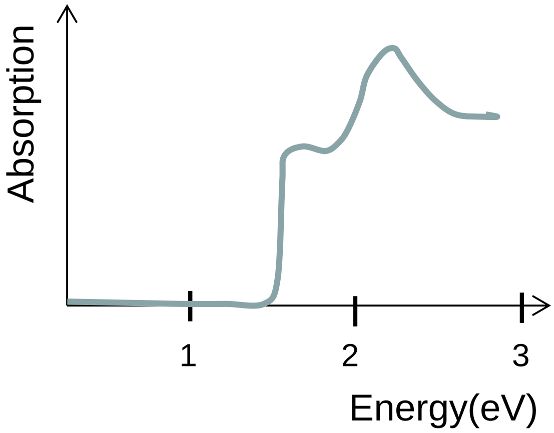
og finn proporsjonalitetskonstanten *C*.

b) Skisser elektron båndstruktur *E*(*k)* for et endimensjonalt system med gitterparameter *a* når en antar et svakt periodisk potensial (nesten fri elektron-tilnærmelsen). Plott de tre laveste energibåndene med *k* langs horisontal akse og *E* langs loddrett akse i en redusert soneframstilling. Forklar hva det periodiske potensialet fører til i forhold til fri elektron modellen.

c) Vi ser nå på et to-dimensjonalt kvadratisk gitter. Figuren viser første Brillouinsone av dette. Vis at den kinetiske energien for et fritt elektron på hjørnet (1) av Brillouinsonen er to ganger den kinetiske energien for et fritt elektron på midtpunktet til sideflaten (2) av Brilloiunsonen. Hvordan blir dette forholdet i tre dimensjoner? Tegn en skisse.



d)



Figuren viser skjematisk et optisk absorbsjonsspektrum fra et materiale.

Hva slags type materiale er dette? Begrunn svaret. Er materialet transparent? Kan du si noe mer om materialet fra denne kurven?

e) Forklar hva som menes med intrinsisk og ekstrinsisk halvleder. Hva menes med n og p doping? Gi eksempel på doping i Si halvleder.

For en intrinsisk halvleder kan en utlede (for temperaturer T som verken er for høye eller lave) følgende uttrykk for konsentrasjonene n og p av elektroner og hull: $np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 \left(m_e m_h\right)^{\frac{3}{2}} \cdot e^{\left(-E_g/k_B T\right)}$ Forklar symbolene. Angi bakgrunn og sentrale antakelser for utledningen av denne likningen, inkludert antakelsen om hvordan energibåndene er. Vi er ikke ute etter en full utledning, men ønsker hovedgangen i utledninga. Kanskje dukker dette integralet opp: $\int_0^\infty x^{\frac{1}{2}} e^{-x} dx = \frac{\sqrt{\pi}}{2}$.

Hva er sammenhengen mellom bølgebølgevektoren for et hull i valensbåndet og bølgevektoren for elektronet som var eksitert for å lage dette hullet? Begrunn svaret.

Norges teknisk-naturvitenskapelige universitet
Faculty of natural sciences
Department of Physics

English

Contact during exam:
Name: Randi Holmestad
Phone: 93880 / 48170066

EXAM IN COURSE TFY4220 Solid State Physics
Saturday 9th June 2012
Time: 9.00 – 13.00
English text (Norwegian text in front)

Number of pages: 4 (+ 4 for English text)
Deadline for result: 30.06.2012

Allowed utilities:
Alternative C (simple calculator, English dictionary, Rottmann formulas book).

Weight on each problem (used for marking) is given in parentheses.

Problem 1 (20%) Introductory Questions

Reply brief on this task!

a) Explain what a reciprocal lattice is and why we introduce it in solid state physics. What is the mathematical relation between real and reciprocal space?

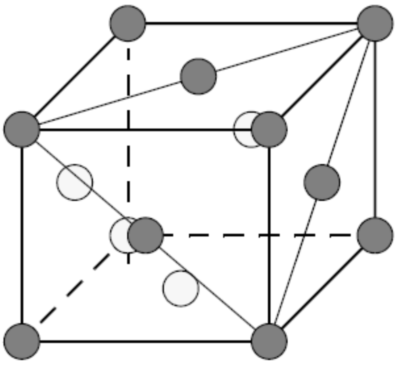
b) What is meant by the heat capacity of a material? What main contributions do we find to the heat capacity? Which parts dominate for the different types of materials?

c) What do we mean by energy bands? What is the cause of energy gaps on materials?

d) What is meant by the Fermi energy? When is the concept of a ‘Fermi surface’ interesting and what is it?

Problem 2 (25%) Structure and Diffraction

a) The figure shows a conventional fcc (face-centered cubic) unit cell with lattice constant *a*. Argue the fcc lattice is a Bravais lattice. Show how this lattice can be regarded as a sc (simple cubic) lattice with a basis consisting of several atoms and provide atomic positions of all atoms in the basis. How can we create a primitive unit cell of the fcc lattice? Draw the primitive cell and give the angles between the primitive unit vectors. What is the volume of the primitive cell?



b) What do we mean by packing fraction? The fcc structure can show what we call ‘closed packer structure’. Explain what this is, how it is realized in the fcc and calculate the packing fraction in this case.

c) The structure factor is given by $S_G = F_{hkl} = \sum_j f_j \exp\left(-i\vec{G}_{hkl}\cdot\vec{r}_j\right)$. Explain all symbols involved and derive of the extinction rules for the fcc structure above.

d) Fluorite CaF_2 is fcc with Ca^{2+} in the corners and center of all surfaces and F^- on the space diagonals ¼ of the diagonal from all corners. Lattice parameter of CaF_2 is a = 5.463 Å at room temperature. Fluorine has an atomic number 9 and calcium number 20. Draw the unit cell and identify the basis of the structure. Set up the S_G for diffraction from CaF_2 expressed by f_{Ca} and f_F for the two ion types, give extinctions for the lowest *hkl* reflections.

e) Calculate the Bragg angle 2θ for the reflections 400, 331 and 420 of fluorite when we have X-ray radiation with wavelength λ= 1.542 Å and specify the order of the strength (intensity) in the three reflections.

Problem 3 (25%) Phonons

Our starting point is a linear lattice with a two-atomic basis. The lattice constant is *a*, and the distance between atoms is *a*/2. The atoms have masses M_1 and M_2. We will study longitudinal waves and assume interactions only between nearest neighbors and that we have harmonic forces. The force constant between nearest neighbors is *C* for the longitudinal oscillation (parallel to the chain).

a) Write down the equations of motion. Assume a wave solution with amplitudes u and v, $u_n = u\cdot e^{i(nKa-\omega t)}$ and $v_n = v\cdot e^{i(nKa-\omega t)}$.

Derive the dispersion relation

$$\omega^2 = C\left[(\frac{1}{M_1}+\frac{1}{M_2})\pm\sqrt{(\frac{1}{M_1}+\frac{1}{M_2})^2-\frac{4}{M_1M_2}\cdot\sin^2\frac{Ka}{2}}\right]$$

We will now study the phonons with light in the infrared (IR) range.

b) Explain why we with IR absorption in crystals generally can only study the central part of Brillouin zone. Find the group velocity ($v = \partial\omega/\partial K$) for the acoustic and optical branch in the limit $K \to 0$ for the linear lattice above.

c) Use the relationship between u and v to say something about the difference between optical and acoustic phonon modes. How are the relationships between neighboring atoms? Explain the difference between transversal and longitudinal modes. For transversal modes the force constant *C* will be generally weaker than for longitudinal modes. Will the speed of sound for longitudinal modes be greater or smaller than for the transversal modes? What is a typical order of magnitude of the sound velocities in solids?

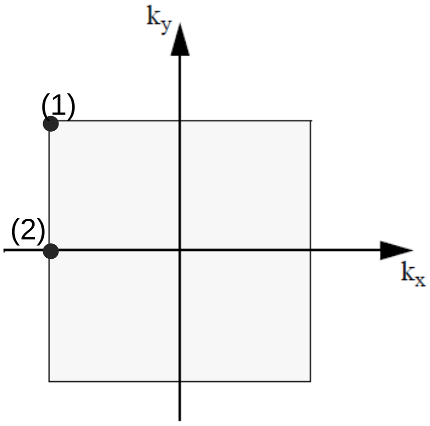
d) In realistic systems it can be difficult to calculate the dispersion relation, and the Debye approximation is widely used. The Debye approximation uses the dispersion relation $\omega = vK$ where v is the speed of sound. Make a sketch and explain what is in this approximation. In order to calculate thermodynamic properties, we need the density of states. Explain how you would proceed to determine the phonon density of states $D(\omega)$ and find $D(\omega)$ in the Debye approximation in the one-dimensional case. Despite the fact that it is a rough approximation, the Debye model gives the correct temperature gradient in the expression for heat capacity. Discuss why.

Problem 4 (30%) Free-electron model, energy bands and semiconductors

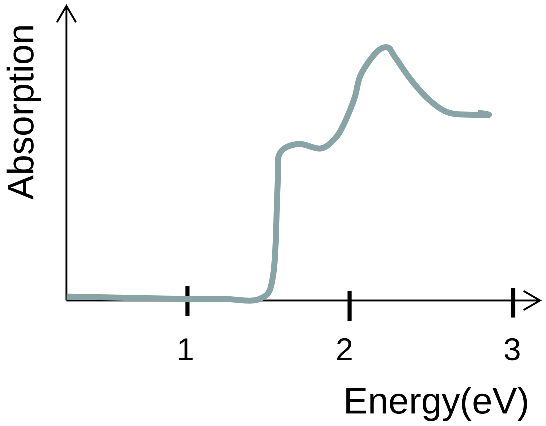
a) Give a brief and qualitative description of free-electron model. We will now study the N free electrons in a cube with edge L. Assume periodic boundary conditions and that the temperature is $T = 0$. Determine the density of k-values in k-space. Define the Fermi energy E_F and show that the expression for the Fermi wave vector can be written as $k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}}$ with volume $V = L^3$. Show that the density of states (number of states per energy unit) $D(E)$ in three dimensions is given by $D(E) = CE^{1/2}$ and find the proportionality constant C.

b) Sketch the electron band structure $E(k)$ for a one-dimensional system with lattice parameter a assuming a weak periodic potential (nearly free electron approximation). Plot the three lowest energy bands with k along the horizontal axis and E along the vertical axis in a reduced zone representation. Explain what the periodic potential leads to in relation to the free electron model.

c) We are now looking at a two-dimensional square lattice. The figure shows the first Brillouin zone of this. Show that the kinetic energy of a free electron on the corner (1) of the Brillouin zone is twice the kinetic energy of a free electron at the center of the side surface (2) of the Brilloiun zone. How will this relationship be in three dimensions? Draw a sketch.



d)



The figure shows schematically an optical absorption spectrum from a material. What type of material is this? Justify your answer. Is the material transparent? Can you say more about the material from this curve?

e) Explain what is meant by intrinsic and extrinsic semiconductor. What is meant by n and p doping? Give an example of doping in Si semiconductor.

For an intrinsic semiconductor, one can derive (for temperatures T that is not too high or low) the following expression for the concentrations n and p of electrons and holes: $np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_e m_h)^{\frac{3}{2}} \cdot e^{\left(-E_g/k_B T\right)}$ Explain the symbols. Give the background and key assumptions for the derivation of this equation, including the assumption of how the energy bands are. We are not looking for a full derivation, but want the main points in the derivation. Perhaps this integral comes up: $\int_0^\infty x^{\frac{1}{2}} e^{-x} dx = \frac{\sqrt{\pi}}{2}$.

What is the relationship between the wave vector for a hole in the valence band and the wave vector of the electron that was excited to make this hole? Justify your answer.

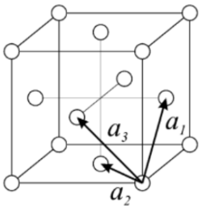
EXAM IN COURSE TFY4220 Solid State Physics
Saturday 8. June 2012
Time: 9.00 – 13.00

DRAFT OF SOLUTION..

Problem 1 (20%) Introductory Questions

Answers of these questions can be found in the text book, and some of them are taken from the introduction questions in the exercises.

Problem 2 (25%) Structure and Diffraction



a) A definition of a Bravais lattice is that all points in the lattice can be reached by translations $\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ with u_1, u_2, u_3 equal integer numbers. We start with the *conventional* unit cell with lattice constant *a*. With a single atom in basis (in (0,0,0)) we can write this fcc lattice as a sc lattice with a basis of 4 atoms placed in

$$r_0 = a(0,0,0),\ r_1 = a\left(\tfrac{1}{2},\tfrac{1}{2},0\right),\ r_2 = a\left(\tfrac{1}{2},0,\tfrac{1}{2}\right),\ r_3 = a\left(0,\tfrac{1}{2},\tfrac{1}{2}\right). \qquad (1)$$

These three last (as vectors) are connecting each corner point with the 'face atoms' (see figure).
A primitive unit cell for the fcc lattice is given by these three vectors,

$$\vec{a}_{1p} = a\left[\tfrac{1}{2},\tfrac{1}{2},0\right],\ \vec{a}_{2p} = a\left[\tfrac{1}{2},0,\tfrac{1}{2}\right],\ \vec{a}_{3p} = a\left[0,\tfrac{1}{2},\tfrac{1}{2}\right] \qquad (2)$$

We can show that the unit vectors for the conventional fcc cell is given as a linear combination of these:

$$\vec{a}_{1c} = \vec{a}_{1p} + \vec{a}_{2p} + \vec{a}_{3p} = a[1,0,0]$$

$$\vec{a}_{2c} = \vec{a}_{1p} + \vec{a}_{3p} - \vec{a}_{2p} = a[0,1,0]$$

$$\vec{a}_{3c} = \vec{a}_{2p} + \vec{a}_{3p} - \vec{a}_{1p} = a[0,0,1]$$

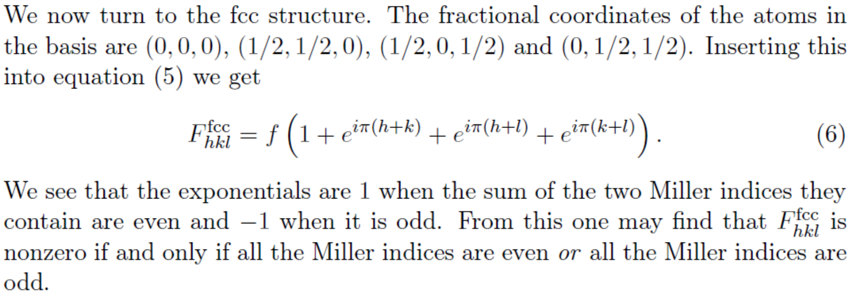
and the fcc lattice therefore has to be a Bravias lattice.
The angles between the primitive vectors in (2) are given by

$$\vec{a}_{1p}\cdot\ \vec{a}_{2p} = \tfrac{\sqrt{2}}{2}\,a\cdot\tfrac{\sqrt{2}}{2}\,a\cdot\cos\theta = \tfrac{1}{4}a^2\text{, giving }\cos\theta = \tfrac{1}{2}\text{ and }\theta = 60^{\circ}$$

The volume of the primitive unit cell is $\frac{a^3}{4}$, which has to be correct since there were 4 atoms in the fcc cell..

b) By packing fraction we mean the maximum proportion of the available volume that can be filled with hard spheres. The fcc structure without a basis (only one atom in the four positions) is a closed packed structure, which means that we have closed-packed layers of spheres placed on the top of each other in a stacking sequence ABCABC.. in the [111] direction in the fcc unit cell (the closed packed layers are (111) planes). To calculate the packing fraction (done in exercise and in the crystallography lab), we have to find the nearest neighbor distance and multiply with number of nearest neighbors. The answer is $\frac{1}{6}\pi\sqrt{2} = 0.74$ which is the densest possible. See Kittel for details.

c) The structure factor is given by $S_G = F_{hkl} = \sum_j f_j \exp\left(-\vec{G}_{hkl} \cdot \vec{r}_j\right)$. Here f_j is the atomic scattering amplitude (form factor) from the individual atom j (these are tabulated), G is a reciprocal lattice vector (between reciprocal lattice points, defining the reflection) and r_j is the coordinate of atom j in the basis. For the simple fcc lattice we will have to sum over the four atoms listed in (1); this is done in exercise 3:

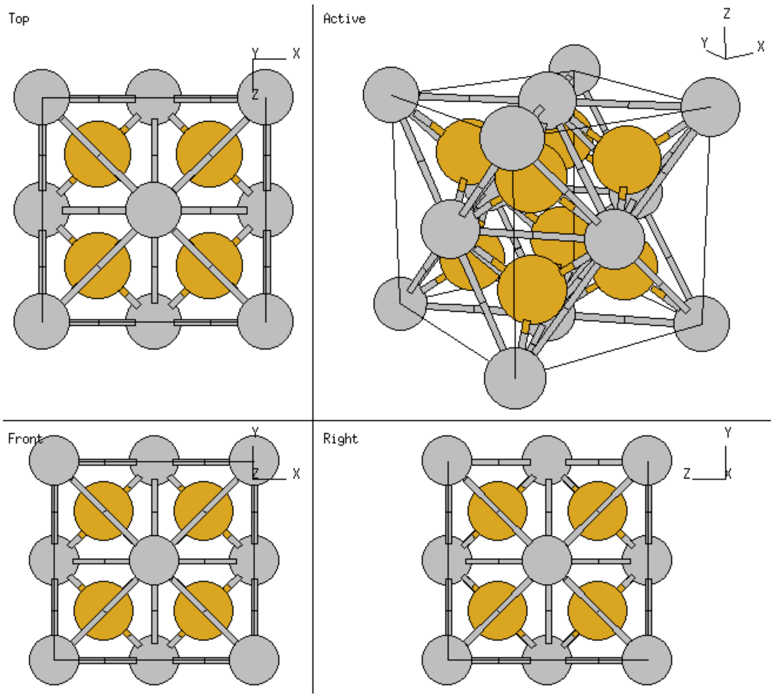


We now turn to the fcc structure. The fractional coordinates of the atoms in the basis are $(0,0,0)$, $(1/2,1/2,0)$, $(1/2,0,1/2)$ and $(0,1/2,1/2)$. Inserting this into equation (5) we get

$$F_{hkl}^{\mathrm{fcc}} = f\left(1 + e^{i\pi(h+k)} + e^{i\pi(h+l)} + e^{i\pi(k+l)}\right). \qquad (6)$$

We see that the exponentials are 1 when the sum of the two Miller indices they contain are even and -1 when it is odd. From this one may find that F_{hkl}^{fcc} is nonzero if and only if all the Miller indices are even *or* all the Miller indices are odd.

d) Drawing of the fluorite structure;



,

Basis is Ca F_2 with coordinates

Ca^{2+} in (0,0,0)
F^- in (¼ , ¼, ¼)
F^- in (- ¼ , -¼,- ¼).

This group repeats in all four Bravais lattice points (0,0,0), (½ ½ 0), (0 ½ ½) and (½ 0 ½)

Structure factor:

If f_{Ca} is the scattering factor for Ca^{2+} and f_F is the scattering factor for F^-.we get

$$S(hkl) =$$
$$\left\{ f_{Ca} + f_F \left[\exp(-2\pi i(h+k+l)/4) + \exp(2\pi i(h+k+l)/4\right]\right\}$$
$$\cdot\left\{1+\exp(2\pi i(h+k)/2+\exp(2\pi i(k+l)/2+\exp(2\pi i(h+l)/2\right\} =$$
$$\left\{ f_{Ca} + 2 f_F \cos(\frac{\pi}{2}(h+k+l))\right\}\cdot\left\{1+(-1)^{h+k}+(-1)^{k+l}+(-1)^{l+h}\right\}$$

Extinction rules are as for fcc: reflections with mixed odd, even *h k l* are absent
All odd or all even gives the last factor equal 4. For mixed indices *h k l* we have 0.

e) Use Braggs law with the given wave length to calculate the angles for 400, 331 and 420, and the expression above to find the structure factors:

Reflection	Angle 2θ (°)	Structure factor
400	68,74	$f_{\mathrm{Ca}}+2f_{\mathrm{F}}$
331	75,93	f_{Ca}
420	78,27	$f_{\mathrm{Ca}}-2f_{\mathrm{F}}$

Since Ca^{2+} has 18 electrons and F^{-} has 10, we have that f_{Ca} is about twice f_{F}.
This will give that 400 is the strongest, 331 somewhat weaker and 420 much weaker.

Problem 3 (25%) Phonons

a) This derivation is done in Kittel pages 97-99 and also in the lecture.

We put up the force on the atom, assuming only nearest neighbour interaction, and then Newton’s second law for each of the two masses in the basis.

$F_{M_1} = C(v_{n-1}-u_n)+C(v_n-u_n)$ and $F_{M_2} = C(u_n-v_n)+C(u_{n+1}-v_n)$. With Newtons 2. law, we get the two coupled differential equations

$M_1\dfrac{\partial^2 v_n}{\partial t^2} = C(u_{n+1}+u_n-2v_n)$ and $M_2\dfrac{\partial^2 u_n}{\partial t^2} = C(v_n+v_{n-1}-2u_n)$

Then we use the solutions $u_n = u\cdot e^{i(nka-\omega t)}$ and $v_n = v\cdot e^{i(nka-\omega t)}$ and get

$$\begin{bmatrix} 2C-M_1\omega^2 & -C(1+e^{-iKa}) \\ -C(1+e^{iKa}) & 2C-M_2\omega^2 \end{bmatrix}\cdot\begin{pmatrix} u \\ v \end{pmatrix} = 0$$

The determinant has to be zero, which gives the equation

$$(2C-M_1\omega^2)(2C-M_2\omega^2)-C^2(1+e^{iKa})(1+e^{-iKa}) = 0$$
$$4C^2-2CM_1\omega^2-2CM_2\omega^2+M_1M_2\omega^4-C^2(1+e^{iKa})(1+e^{-iKa}) = 0$$

This is a second order equation in ω^2,

$$x = \frac{-b\pm\sqrt{b^2-4ac}}{2a}, \quad \begin{aligned} a &= M_1M_2 \\ b &= -2C(M_1+M_2) \\ c &= 2C^2(1+\cos Ka) \end{aligned}$$

$$\omega^2 = \frac{2C(M_1+M_2) \pm \sqrt{4C^2(M_1+M_2)^2 - 4M_1M_2 2C^2(1+\cos Ka)}}{2M_1M_2}$$

………….

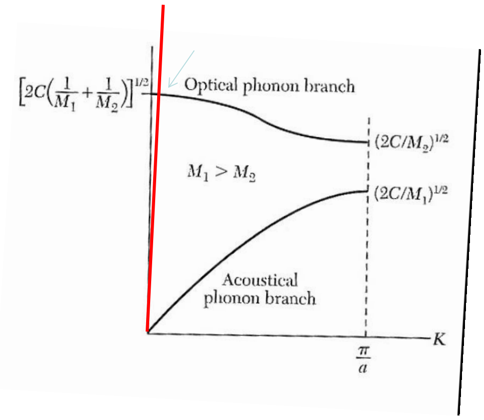
and gives the dispersion relationship

$$\omega^2 = C\left[\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm \sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4}{M_1M_2}\cdot\sin^2\frac{Ka}{2}} \right]$$

b) This was done in the lab exercise on lattice vibrations, from there we have:

> Absorption of a photon and the creation of a phonon in a crystal requires that energy and momentum are conserved, that is $\hbar\omega_{\text{phonon}} = \hbar\omega_{\text{photon}}$ and $\hbar k_{\text{phonon}} = \hbar k_{\text{photon}}$. A typical wavenumber of an IR-photon is $k \simeq 10^5\,\text{m}^{-1}$. This is a very small value compared to edge of the Brillouin zone which lies at $k = \frac{2\pi}{a} \simeq 10^{10}\,\text{m}^{-1}$ for a typical value of the lattice constant a. We can therefore only study the very centre of the Brillouin zone directly by IR spectroscopy.

The red line in the figure to the right represents $h\omega_{photon}$



Group velocity for the optical and acoustic mode:

Optical mode: $\frac{d\omega}{dk} = 0$

Acoustic mode: $\frac{d\omega}{dk} = a\sqrt{\frac{1}{2}C\left(\frac{1}{m_1+m_2}\right)}$

c) For the acoustic wave we find that $\frac{u}{v} = 1$ and for the optical $\frac{u}{v} = -\frac{M_2}{M_1}$, $K \to 0$.

This tells us that both masses oscillate in same direction with same amplitude (neighboring atoms oscillates in phase). For the optical band they oscillate in opposite directions, the lightest atom with largest amplitude. Since the group velocity for these waves is zero, we can think of it as a standing wave. Centre of mass is not moving. Such oscillations are excited with opposite effect on the two atoms – with an ion crystal with opposite charge of the two atoms, EM radiation will excite this mode (give rise to an electric dipole moment - oppositely charged planes plans will vibrate against each other)– therefore it is called optical.

Transverse and longitudinal modes – see fig 10 page 98 in Kittel.

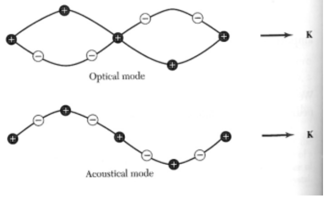
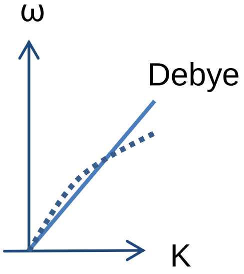


Figure 10 Transverse optical and transverse acoustical waves in a diatomic linear lattice, illustrated by the particle displacements for the two modes at the same wavelength.

The transversal velocity of sound will be smaller than the longitudinal. The magnitudes of sound velocities are around a few thousand meters per second. For SiC in the lab we found ~10.000 m/s and ~7000 m/s for the two optical modes (transversal lower than longitudinal). SiC is very hard and have a relatively large v. for copper it is ~4700 m/s, polyethylene is ~1900 m/s and Plexiglas is ~1700 m/s.

c) The Debye approximation assumes a linear dispersion relation, and assumes that the acoustic mode is dominating. The sound velocity is assumed constant independent of polarization type. Density of states can be found by applying periodic boundary conditions over N primitive cells, find that interval between successive K values $\Delta K = \left({2\pi}/{L} \right)$ in K space. Number of modes for dK is $\left({L}/{2\pi} \right) \cdot dK$ which gives $\left({L}/{\pi} \right) \cdot \frac{d\omega}{{d\omega}/{dK}}$ and the answer is $D(\omega) = \left({L}/{\pi} \right) \cdot \frac{1}{v}$ which gives a dependence of D with ω^{-1}



(For 3D:
find the total number of modes with wavevector less than allowed K is found to be $\left({L}/{2\pi} \right)^3$ times the volume of a sphere with a radius K: $N = \left({L}/{2\pi} \right)^3 \left({4\pi K^3}/{3} \right)$ To find the density of states we use this expression, $D(\omega) = \frac{dN}{d\omega} = \frac{VK^2}{2\pi^2} \left(\frac{dK}{d\omega} \right)$ In this we could put in the Debye approximation; $\omega = vK$ $D(\omega) = \frac{V \frac{\omega^2}{v^2}}{2\pi^2} \left(\frac{1}{v} \right) = \frac{V\omega^2}{2\pi^2 v^3}$
This gives a quadratic dependence of D with ω.)

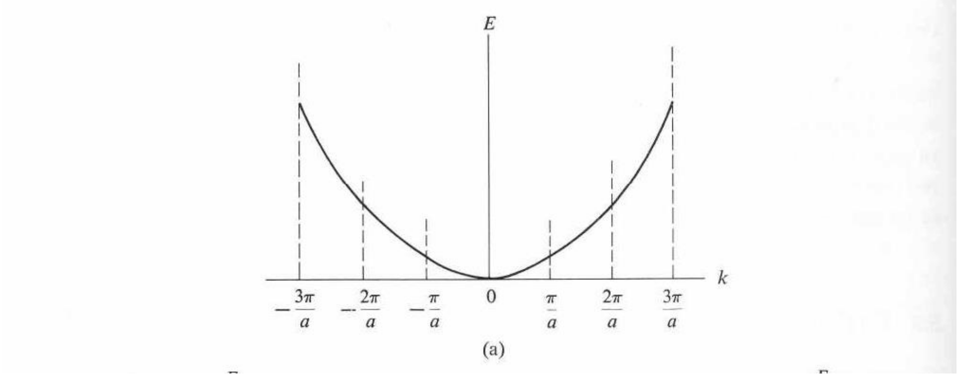
With the Debye-approximation we keep this dependence up to a maximum frequency ω_D, with a corresponding cutoff wave vector $K_D = {\omega_D}/{v} = \left({6\pi^2 N}/{V} \right)$.The Debye model gives a T^3 dependence of the heat capacity for low T and a makes a heat capacity approach a constant for high T. The T^3 dependence for low T can be explained qualitatively by all phonon modes of a wave vector less than a given K have a thermal energy $k_B T$, and all over (up to K_D) are not excited, giving that the fraction excited are proportional to T^3 - an energy U proportional to T^4 and a heat capacity proportional to T^3. See figure 10 page 115 in Kittel. For high T the heat capacity approaches the classical value of $3Nk_B$.

Problem 4 (30%) Free-electron model, energy bands and semiconductors

a) Free electron model: 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 L*L*L=L^3 =V in real space; which is $\left(\frac{2\pi}{L}\right)^3$. There is one allowed wave vector for each $\left(\frac{2\pi}{L}\right)^3$ this will then give:

$$N = 2\frac{\frac{4}{3}\pi k_F^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{k_F^3 V}{3\pi^2} \text{ which}$$

gives $k_F = \left(\frac{N3\pi^2}{V}\right)^{1/3}$.



This gives the Fermi energy

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3N\pi^2}{V}\right)^{2/3}.$$

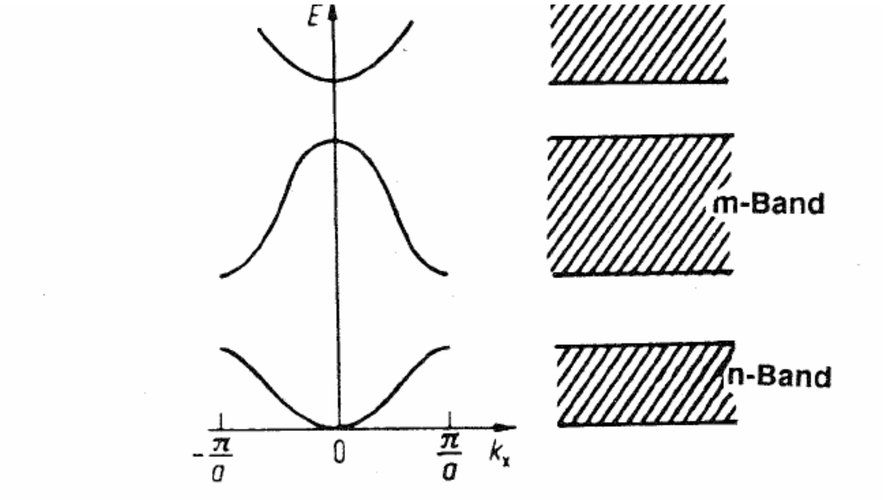
From this expression we can now find the number of states less than *E*, given by *N(E):*

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3N(E)\pi^2}{V}\right)^{2/3} \quad \text{gives} \quad N(E) = \frac{V}{3\pi^2}\left(\frac{E2m}{\hbar^2}\right)^{3/2}$$

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

This gives $C = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}$

b) A weak periodic potential leads to energy gaps at the Brillouin zones. In a reduced zone representation this will look for example like this:



We get energy bands for the electrons separated with forbidden energy gaps.

c) From exercise 8:

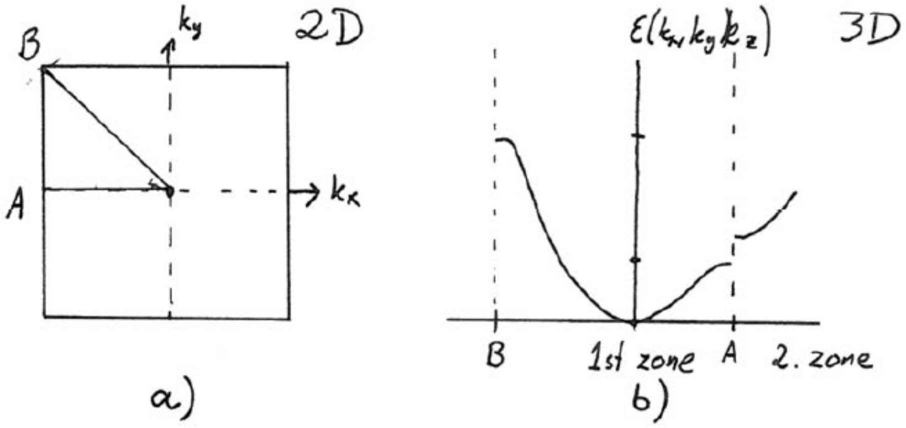
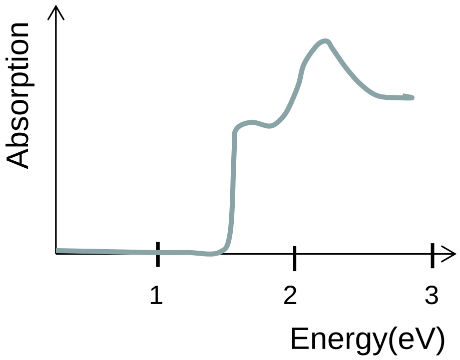


Figure 1: a) The first Brillouin zone in 2D b) The energy plot allong center to side edge and center to corner in 3D.

a) The wavevector at the corner is longer than the wavevector at the midpoint of a side by the factor $\sqrt{2}$. As $\varepsilon \propto k^2$ for a free electron, the energy is higher by $\left(\sqrt{2}\right)^2 = 2$.

b) In three dimensions the energy at a corner is higher by $\left(\sqrt{3}\right)^2 = 3$ than at the midpoint of a face.

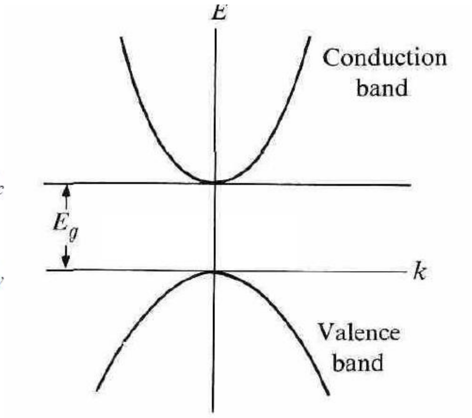


d)

The material studied is a semiconductor with band gap about 1,5 eV, this we see since there is no absorption of phonons with energies less than 1,5 eV. The material is transparent for energies less than 1.5 eV. This is in the IR region and not in the visible region. It will therefore not look transparent.

The details of the start of the absorption (not an abrupt edge, but a small ‘bend’ at the bottom to the left) tell us that this is an indirect semiconductor. Also the wiggles to the right gives us information about other interband transitions.

e)
Intrinsic: undoped, no states in band.
Extrinsic: doped, energy level of impurity states in band gap
p-doping: empty states near the top of the valence band
n-doping: filled electron states near the bottom of the conduction band
Explained in Kittel page 209-213.



We assume a empty conduction band and a filled valence band.

Assuming the free electron model we have for the valence band $E = E_V - \frac{\hbar^2}{2m_h}k^2$ and for the conduction band $E = E_C - \frac{\hbar^2}{2m_e}k^2$ with effective masses..

Expression for the density of states *D(E)*:

$$D(E) = \frac{V}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}\left(E - E_C\right)^{\frac{1}{2}}$$ (this can be taken from problem 4 a) .

We can do this $f_e(E) = \frac{1}{e^{(E-\mu)/k_BT}+1} \approx e^{-(E-\mu)/k_BT}$ because the band gap in semiconductors (~1 eV) is usually much larger than k_BT and therefore $(E-\mu) >> k_BT$.

Concentration *n* of electrons in the conduction band:

$$n = \frac{N}{V}\int_{E_C}^{\infty} f(E)\cdot D(E)dE = \frac{1}{V}\int_{E_C}^{\infty} e^{-(E-\mu)/k_BT}\cdot\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left(E-E_C\right)^{\frac{1}{2}}dE$$

$$n = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} e^{\frac{\mu}{k_BT}}\int_{E_C}^{\infty} e^{-E/k_BT}\cdot\left(E-E_C\right)^{\frac{1}{2}}dE$$

This was done in the lectures and in Kittel on page 206.

We have to use the integral $\int_0^\infty u^{\frac{1}{2}} e^{-u} du = \frac{\sqrt{\pi}}{2}$

The answer becomes:

$$n = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} e^{\frac{(\mu - E_C)}{k_B T}}$$

In the same way we can find *p* to be equal to $p = 2\left(\frac{m_p k_B T}{2\pi\hbar^2}\right)^{3/2} e^{\frac{(E_V - \mu)}{k_B T}}$.

When we set up the product *pn*, μ will disappear, and with $E_g = E_C - E_V$ we get the given formula - $np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 \left(m_e m_h\right)^{\frac{3}{2}} \cdot e^{\left(-E_g / k_B T\right)}$, this shows the T dependence of the charge density concentration.

The relationship between the wave vector for a hole in the valence band and the wave vector of the electron that was excited to make this hole is $\vec{k}_h = -\vec{k}_e$.

The total wave vector of a filled band is $\vec{k}_{tot} = 0$. The remaining hole when an electron is removed must have its wave vector in the opposite direction of the electron due to momentum conservation.