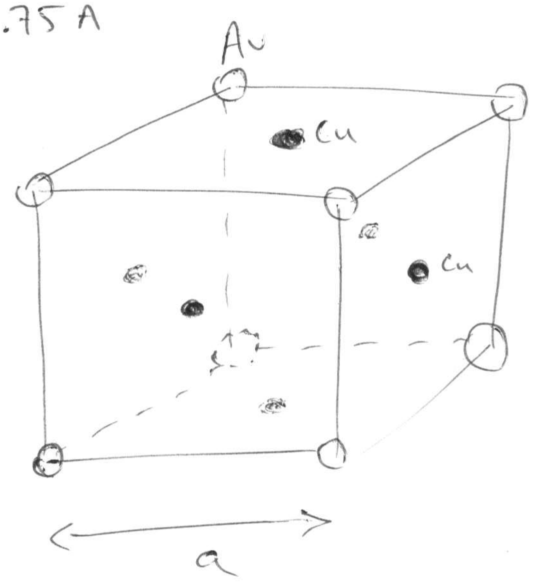
Exam 2009-06-17

Condensed Matter Physics I

Problem 1 Given: Cu, fcc

Alloy: replace corners in unit cell by Au

$\Longrightarrow a = 3.75\,\text{Å}$



Wanted: a) Crystal structure:

b) Chemical composition:

Cu_3Au

since fcc contains 4 at/cell

corners (Au) $\Longleftrightarrow 8 \times \frac{1}{8} = 1$ at/cell

c) Density:

$$\rho = \frac{3m_{Cu} + m_{Au}}{V} = \frac{3 \cdot 63.55\,u + 196.97\,u}{a^3} =$$

$$= \frac{387.47\,u \cdot 1.66 \cdot 10^{-27}\,kg/u}{(3.75 \cdot 10^{-10}\,m)^3} = \underline{12.2\ g/cm^3}$$

d) The coordination number of the Au atoms is 12:

(this is true for all atoms in the structure, i.e., for fcc)

An Au-atom has 4 neighboring Cu atoms in the same z-plane, 4 below and 4 above. $\Sigma 12$

One could also see it this way:

In the cell, the Au atom in the corner has 3 neighboring Cu-atoms on the connected surfaces.

The contribution from this cell is thus $3 \times \frac{1}{2}$

surface factor

The corner atom is corner for 8 cells

$\Longrightarrow \quad 8 \times 3 \times \frac{1}{2} = 12$ nearest neighbors

Problem 2

Given: Al: 3 val. el./atom $a = 4.05\,\mathring{A}$

a) Show: $\varepsilon_F = 11.7\,eV$

Solution: Assume free el. model $\varepsilon_F = \frac{\hbar^2 (3\pi^2 n)^{2/3}}{2m}$

$$n = \frac{\#\text{ free el.}}{\text{Vol}} = \frac{3\ {}^{el}/_{atom} \cdot 4\ {}^{at}/_{cell}}{a^3} \longrightarrow \text{fcc}$$

$$\Rightarrow \varepsilon_F = \frac{\hbar^2 \cdot (36\pi^2)^{2/3}}{2ma^2} = \frac{(1.055\cdot 10^{-34})^2 \cdot (36\pi^2)^{2/3}}{2\cdot 9.11\cdot 10^{-31}\cdot (4.05\cdot 10^{-10})^2}[J] \cdot \frac{1\,[eV]}{1.602\cdot 10^{-19}\,[J]} =$$

$$= 11.66\,eV \approx \underline{\underline{11.7\,eV}}$$

b) Given: Resistivity $\rho_{Al} = 2.45\,\mu\Omega cm$

Estimate: Mean free path for cond. el in Al

Solution: $\sigma = \frac{ne^2\tau}{m} = \frac{1}{\rho_{Al}}$; $\tau = \frac{l}{v_F}$; $v_F = \sqrt{\frac{2\varepsilon_F}{m}}$

$$\Rightarrow l = v_F \tau = \sqrt{\frac{2\varepsilon_F}{m}} \cdot \frac{m}{\rho_{Al}\cdot ne^2} = \sqrt{2m\varepsilon_F} \cdot \frac{1}{\rho_{Al}\cdot ne^2} = \{\text{above}\} =$$

$$= \frac{\hbar\cdot(3\pi^2 n)^{1/3}}{\rho_{Al}\cdot ne^2} = \frac{\hbar\,(3\pi^2)^{1/3}}{\rho_{Al}\cdot e^2\cdot\left(\frac{12}{a^3}\right)^{2/3}} = \{\rho_{Al} = 2.45\cdot 10^{-8}\,\Omega m\} = \underline{\underline{16\,nm}}$$

c) Discuss: Relation between defects and resistivity. Why is $\rho_{Al,pure} \neq 0$?

Solution: $\rho(T) = \rho_{ideal}(T) + \rho_{imp}$ $\rho_{imp} \propto$ # of impurities (point defects)

from interaction with lattice vibrations (phonons)

These phonons act as scattering particles

Electrons scatter on all different kind of impurities, crystal defects, but not on the perfect lattice

(Al becomes superconducting below 1.2 K due to the el-phonon interaction and ρ goes to zero)

Problem 3

Given: X-ray, $\lambda = 1.5405\,\text{Å}$, body-centered tetragonal

Four lowest Bragg angles : $\theta = 21.00°, 22.06°, 28.78°, 32.09°$

a) Wanted: $\bar{G}(hkl)$ for tetragonal lattice $(a\hat{x}, a\hat{y}, c\hat{z})$

Solution: $\bar{G}(hkl) = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$ where

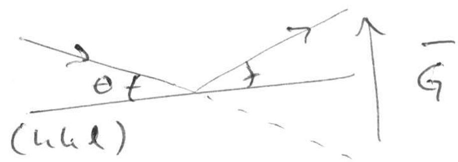
$$\bar{b}_1 = 2\pi \frac{\bar{a}_2 \times \bar{a}_3}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)} = 2\pi \frac{ac\,\hat{x}}{a^2 c} = \frac{2\pi}{a}\hat{x}$$

$$\bar{b}_2 = \dots = \frac{2\pi}{a}\hat{y} \quad ; \quad \bar{b}_3 = \frac{2\pi}{c}\hat{z}$$

b) Given: Diffraction condition $\Delta k = \bar{G}$

Wanted: Quadratic form for tetragonal lattice

Solution: $|\bar{k}| = \frac{2\pi}{\lambda}$



$$2|\bar{k}|\sin\theta = |\bar{G}|$$

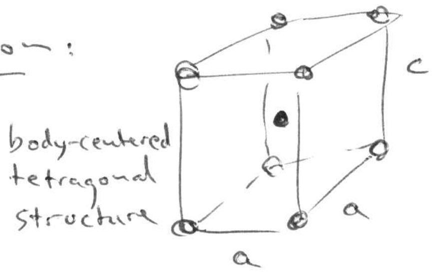
Square: $2^2\left(\frac{2\pi}{\lambda}\right)^2 \sin^2\theta = |\bar{G}|^2 = (2\pi)^2\left(\left(\frac{h}{a}\right)^2 + \left(\frac{k}{a}\right)^2 + \left(\frac{l}{c}\right)^2\right)$

$$\Longrightarrow \quad \sin^2\theta = \frac{\lambda^2}{4a^2}\left(h^2 + k^2 + \left(\frac{a}{c}\right)^2 l^2\right)$$

c) Given: bcc : $h+k+l$ = even for reflex

Motivate: This applies also to body-centered tetragonal structure

Solution:



Structure factor

$$S = \sum_j f_j e^{i\bar{G}\cdot\bar{r}_j} = \left\{ \begin{array}{l}\text{basis of 2 atoms} \\ \text{at } \bar{0} \text{ and } \left(\frac{a}{2}, \frac{a}{2}, \frac{c}{2}\right)\end{array}\right\}$$

$$= f\cdot\left(e^0 + e^{i\bar{G}\cdot\left(\frac{a}{2},\frac{a}{2},\frac{c}{2}\right)}\right) = f\left(1 + e^{i\bar{G}\cdot\left(\frac{\bar{a}_1+\bar{a}_2+\bar{a}_3}{2}\right)}\right)$$

$$= f\cdot\left(1 + e^{i(h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3)\left(\frac{\bar{a}_1+\bar{a}_2+\bar{a}_3}{2}\right)}\right) \overset{\bar{a}_i \bar{b}_j = 2\pi\delta_{ij}}{=} f\left(1 + e^{i\pi(h+k+l)}\right) = \begin{cases} 2f & \text{even sum} \\ 0 & \text{odd sum}\end{cases}$$

Note: We do not need to know the expressions for $\bar{b}_i$ only that $\bar{a}_i \cdot \bar{b}_j = 2\pi\delta_{ij}$

Problem 3...

d) Index the structure and determine a and c. $\lambda = 1.5405\ \text{Å}$

Solution: Index means to find $(h\,k\,l)$ for the measured angles.

Use result from b): $\sin^2\theta = \frac{\lambda^2}{4a^2}\left(h^2+k^2+\left(\frac{a}{c}\right)^2 l^2\right)$

Index	θ (°)	$\sin^2\theta$	$(h\ k\ l)$	Equation	Result
1	21.00	0.12843	(011), (101)	$\sin^2\theta = \frac{\lambda^2}{4a^2}\left(1+\left(\frac{a}{c}\right)^2\right)$	$\sin^2\theta = 0.12848$
2	22.06	0.14106	(110)	$\sin^2\theta = \frac{\lambda^2}{4a^2}\cdot 2$	$a = 2.900\ \text{Å}$
3	28.78	0.23179	(002)	$\sin^2\theta = \frac{\lambda^2}{4c^2}\cdot 4$	$c = 3.200\ \text{Å}$
4	32.09	0.28223	(200), (020)	$\sin^2\theta = \frac{\lambda^2}{4a^2}\cdot 4$	$a = 2.900\ \text{Å}$

The two lowest indices should be (110) and (011) and the two highest (200) and (002) (even sum h+k+l)

Note that (011) involves both a and c but (200) and (002) involves only a or c. It is likely that index 2 only involves a, i.e, that it is the reflex (110), since $\frac{(\sin^2\theta)|_4}{(\sin^2\theta)_2} \approx 2$

With this observation the indices are found.

An equation can then be written for each index.

2 and 4 gives $\underline{\underline{a = 2.900\ \text{Å}}}$ and 3 gives $\underline{\underline{c = 3.200\ \text{Å}}}$.

Index 1 can be verified for instance by calculating $\sin^2\theta$ from obtained a and c. $\Rightarrow$ $\sin^2\theta = 0.12848$, $\theta = 21.005°$

which is very close to measured angle.

Problem 4

Given : Transversal, optical lattice vibrations, $f = 9 \cdot 10^{12}$ Hz
independent of λ and prop. direction.
Diamond structure, $a = 5.66$ Å

a) Wanted : Average number of such phonons in a 1 cm^3 crystal at room temp.

Solution : In a crystal with N atoms (primitive cells) there are N vibration modes per polarization direction.

Each vibration mode contains a number of phonons

$$n(\omega) = \frac{1}{e^{\hbar\omega/k_BT} - 1} \quad \text{phonons/mode}$$

$$\Rightarrow \#\text{phonons} = n(\omega) \cdot \underbrace{\#\text{cells}}_{V/a^3} \cdot \underbrace{\frac{\#\text{at}}{\text{cell}}}_{8 \text{ for diamond}}$$

(2 x 4 for fcc)

$\hbar\omega = hf$

$$\frac{\hbar\omega}{k_BT} = \frac{\hbar}{k_B} \cdot \frac{2\pi \cdot 9 \cdot 10^{12}\, s^{-1}}{300 \quad K} = 7.64 \cdot 10^{-12}\, Ks \cdot \frac{2\pi \cdot 9 \cdot 10^{12}}{300} \frac{s^{-1}}{K} = \underline{1.44}$$

$$\Rightarrow n(\omega, \text{room temp}) = 0.31 \Rightarrow \#\text{phonons} = 0.31 \cdot 8 = \underline{2.48/\text{cell}}$$

$$\#\text{cells} = \frac{(1\,cm)^3}{(5.66 \cdot 10^{-8}\,cm)^3} = 5.5 \cdot 10^{21} \Rightarrow \text{total } \#\text{phonons} = 1.4 \cdot 10^{22}$$

in one cm^3

b) Calculate: Thermal energy associated with these vibrations

Solution : $\langle \varepsilon \rangle = \underbrace{\hbar\omega}_{hf} \cdot \langle n \rangle = 6.63 \cdot 10^{-34}\, J \cdot s \cdot 9 \cdot 10^{12} s^{-1} \cdot 1.4 \cdot 10^{22}\, cm^{-3} =$

$= 83.5\, J/cm^3$ (or 11.8 meV/atom)

Problem 4...

c) Estimate contribution from lattice vib. to specific heat at room temperature

Solution:

$$C_v = \frac{\partial U}{\partial T} \approx \frac{\Delta U}{\Delta T} = \frac{\Delta n(\omega)}{\Delta T} \cdot \hbar\omega \cdot \#\text{cells} \cdot \frac{\#\text{at}}{\text{cell}}$$

$\hbar\omega$: $6.63 \cdot 10^{-34}\,\text{J s} \cdot 9 \cdot 10^{12}\,\text{s}^{-1}$

$\#\text{cells}$: $5.5 \cdot 10^{21}\,\text{cm}^{-3}$

$\frac{\#\text{at}}{\text{cell}}$: 8

Let $\Delta T = 1\,\text{K}$

$$\Rightarrow \Delta n(\omega) = n(300\,\text{K}) - n(299\,\text{K}) = 0.3104 - 0.3085 = 1.95 \cdot 10^{-3}$$

$$\Rightarrow \underline{\underline{C_v = 0.51\ \text{J}/\text{cm}^3\,\text{K}}}$$

Problem 5

a) Discuss: four different experiments that can be used to study semiconductors. * How exp. is performed
* Obtained information

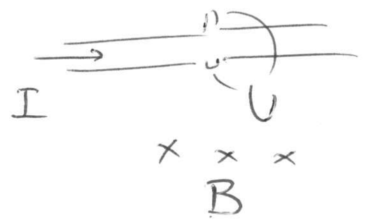
Solution: ① Resistivity measurement as a function of temp. (resistance)

Send current through sample, measure voltage

vary the temperature

Obtained info: E_g (intrinsic $\sigma \sim \frac{1}{\rho} \sim e^{-E_g/2k_BT}$)

② Hall effect measurements



Measure voltage perpendicular to current and magnetic field.

Obtained info: Sign and number of carriers

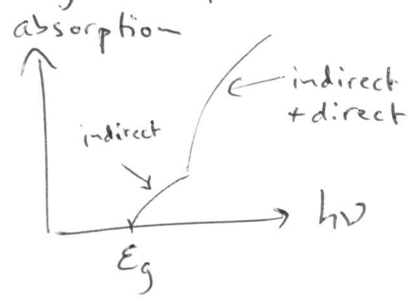
$$R_H = \frac{E_y}{j_x B} = -\frac{1}{(n-p)e}$$

③ Optical absorption

Send light of variable wavelength through sample.

Study absorption / transmitted light.

Obtained info: E_g, direct or indirect bandgaps



④ Seebeck effect:

Create a temp. gradient and measure voltage.

Obtained info: type of doping (n/p)

⑤ Haynes-Shockleys experiment

Excite carriers with a laser, let the excited carriers drift in an electric field + detect with oscilloscope.

Obtained info: ambipolar mobility, type of carriers

Problem 5

b) Wanted: Can effective mass of a certain Bloch state be both positive and negative?

- In two-dim. crystals?
- — " — one — " —

Solution: A Bloch state has a given $\bar{k}$-vector and we want to see if the effective mass

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k^2} \quad \text{is negative or positive}$$

In one dimension $\frac{1}{m^*}$ is given as above and has to be either pos or negative

In two dimensions the effective mass becomes a tensor

$$\left(\frac{1}{m^*}\right)_{\mu\nu} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\bar{k})}{\partial k_\mu \partial k_\nu} \qquad \mu, \nu \in (x, y)$$

This property will depend on direction in general and can be both positive and negative at the same time, at the given point $\bar{k}$.

Problem 6

a) Given: Free spin paramagnet, $J = 1/2$

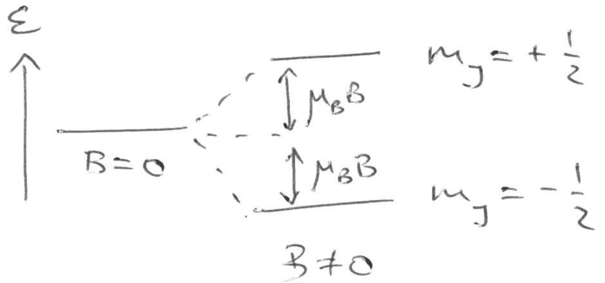
Show: How to obtain Curie law: $\chi \propto \frac{1}{T}$

Solution: Magnetic moment $\bar{\mu} = -g\mu_B \bar{J}$

Energy in magnetic field: $U = -\bar{\mu} \cdot \bar{B} =$

$= m_J g \mu_B B = \pm \frac{1}{2} \cdot 2\mu_B B$

$(m_J = -J \ldots, +J = \pm \frac{1}{2})$



Let N_1 spins of energy $-\mu_B B$
N_2 — " — $+\mu_B B$
$\Big\} \; N_1 + N_2 = N$ (number of magnetic moments in the solid)

Bolzmann statistics:

$$\frac{N_1}{N} = \frac{e^{-(-\mu_B B)/k_B T}}{e^{-\mu_B B/k_B T} + e^{+\mu_B B/k_B T}} = \left\{ \text{put } x = \frac{\mu_B B}{k_B T} \right\} = \frac{e^x}{e^x + e^{-x}}$$

$$\frac{N_2}{N} = \frac{e^{-x}}{e^x + e^{-x}} \qquad M = \mu_B (N_1 - N_2) = \mu_B N \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

For small fields (paramagnetic response): $x \ll 1$

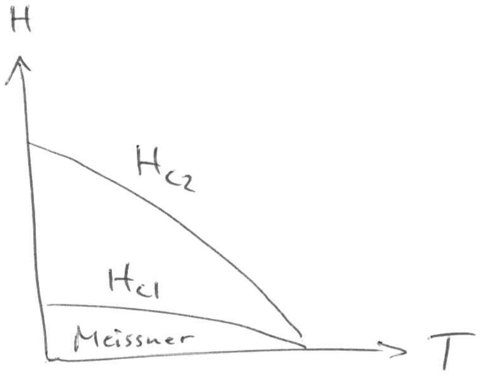
$$M \approx \mu_B N \frac{1 + x - (1 - x)}{1 + x + 1 - x} = \mu_B N \cdot x = \frac{\mu_B^2 B}{k_B T}$$

$$\chi = \frac{M}{H} = \frac{M}{B} \cdot \mu_0 = \mu_0 \mu_B^2 N \cdot \frac{1}{k_B T} \propto \frac{1}{T}$$

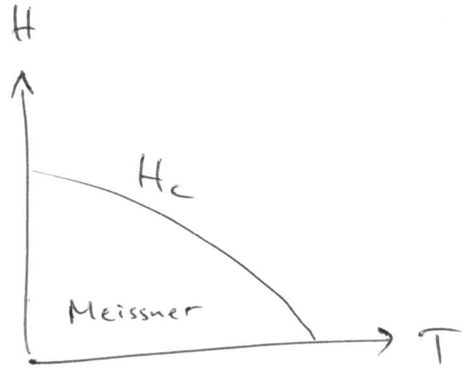
Problem 6b

Describe magnetic response of type-I and type-II superconductors.

Solution



type-II

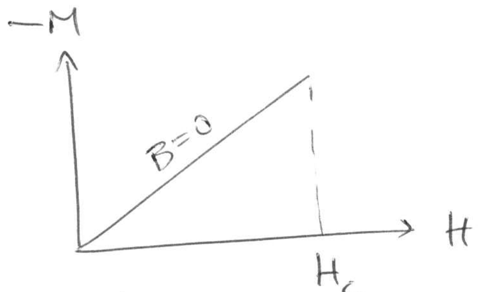


type-I

In type-I superconductors, disregarding shape-effects, magnetic field is expelled up to the critical field H_c.

$\Longrightarrow$ "perfect diamagnetic" with $M = -H$, $B = 0$

Meissner state.



type-I

In type-II superconductors, there is a lower critical field, H_{c1}, up to which the Meissner state is preserved. Above this field, vortices penetrate the superconductor and reduce the diamagnetic response. Superconductivity is destroyed at H_{c2}.