Examination in Condensed Matter Physics I, FK3004, 7.5 hp
Friday, March 25, 2011, 09.00-14.00.

Solutions

Allowed help:
- periodic table and fundamental constants (distributed)
- formula sheet (distributed)
- pocket calculator, BETA / mathematics handbook or similar

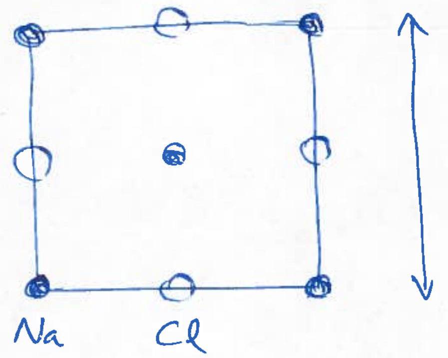
Instructions:
All solutions should be easy to read and have enough details to be followed. The use of nontrivial formulas from the formula sheet should be explained. *Summarize each problem* before its solution, so that the solution becomes self-explained. State any assumptions or interpretation of a problem formulation.

Good luck! / A.R.

1. The sodium chloride (NaCl) structure can be described using an *fcc* lattice with a basis of two ions at **0** and $(a/2)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$, respectively. Assume that the ions can be regarded as impenetrable spheres with definite radii r_{Na} and r_{Cl}.
a) Make a simple sketch of the ion arrangement in the (100) plane. Express the nearest neighbor distance as a function of lattice parameter a. (1p)
b) Given $r_{\mathrm{Na}} = 0.95$ Å and $r_{\mathrm{Cl}} = 1.81$ Å, verify that the Cl ions make contact only with the Na ions and calculate the lattice parameter for NaCl. (1.5p)
c) A simple cubic structure has a filling fraction of 52 %. Find the corresponding filling fraction for NaCl. (1.5p)

See Exam 2008-06-05, problem 1.

a)



Nearest neighbor distance is $\frac{a}{2}$

b) $2(r_{Na} + r_{Cl}) > \sqrt{2}\,(r_{Cl} + r_{Cl})$ OK

$a = 5.52$ Å

c) $f = 68\%$

2. Metallic sodium (Na) has a density $d = 0.97\,\mathrm{g/cm^3}$, a resistivity $\rho = 4.2\,\mu\Omega\mathrm{cm}$ and one conduction electron per atom. Sodium is fairly well described by the free electron model. Assume that an electrical field of $1\,\mathrm{V/cm}$ is applied to drive a current through a piece of sodium. The field will shift the Fermi sphere by an amount Δk. Find the ratio $\Delta k/k_F$, where k_F is the radius of the Fermi sphere. (4p)

Solution: $\Delta\bar{k} = \langle \bar{k} \rangle$

With drift velocity $\bar{v}_d$, we have $\hbar\langle\bar{k}\rangle = m\bar{v}_d$

$$\Longrightarrow \Delta\bar{k} = \frac{m\bar{v}_d}{\hbar}$$

v_d is obtained from $\bar{j} = -ne\bar{v}_d = \sigma E = \frac{1}{\rho}E$

$$\Longrightarrow \Delta\bar{k} = -\frac{m\bar{E}}{\hbar ne\cdot\rho}$$

For free electrons: $k_F = (3\pi^2 n)^{1/3}$

$$\left[\frac{\Delta k}{k_F} = \frac{mE}{\hbar\rho\cdot e\,(3\pi^2)^{1/3}\cdot n^{4/3}}\right]$$

$$n = \frac{d\cdot N_A}{M_{Na}} = \frac{0.97\,\cancel{g}/cm^3 \cdot 6.022\cdot10^{23}\,\cancel{mol}}{22.99\,\cancel{g}/\cancel{mol}} = 0.254\cdot10^{23}\,(cm)$$

or: $\frac{2}{a^3}$ ← bcc

$$\Longrightarrow k_F = 9.1\cdot10^{7}\,cm^{-1}$$

$$\Delta k = \frac{9.109\cdot10^{-31}(kg)\cdot 1\,[V/cm]}{1.055\cdot10^{-34}[Js]\cdot0.254\cdot10^{23}[cm^{-3}]\cdot1.602\cdot10^{-19}[C]\cdot4.2\cdot10^{-6}[\Omega c}$$

$$\Delta k = 5.05\cdot10^{5}\left(\frac{kg\cdot\frac{V}{\cancel{cm}}\cdot cm^{3}}{J\cdot s\cdot C\cdot\Omega\cdot\cancel{cm}}\right) = \left(\frac{\cancel{kg}\cdot\cancel{V}\cdot cm}{\cancel{kg}\left(\frac{m}{s^2}\right)\cdot m\cdot\cancel{A}\cdot\cancel{V}/}\right)$$

$10^{-2}\,m^{-1}$
$= 10^{-4}\,cm^{-1}$

$\Delta k = 50.5\,cm^{-1}$

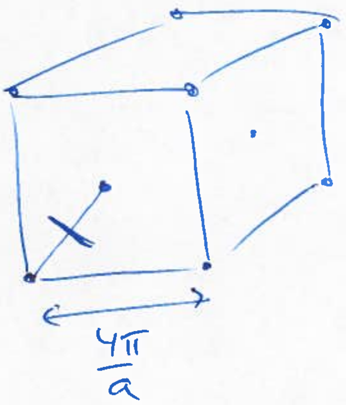
$$\Longrightarrow \frac{\Delta k}{k} = \underline{\underline{5.55\cdot10^{-7}}}$$

3. a) Show that the volume v_g of the reciprocal lattice primitive cell is $v_g = (2\pi)^3/v_c$, where v_c is the volume of the direct lattice primitive cell. Hint: $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = (\mathbf{A} \cdot \mathbf{C})\mathbf{B} - (\mathbf{A} \cdot \mathbf{B})\mathbf{C}$. (1.5p)
b) Describe what a Brillouin zone is. (1p)
c) Iron (Fe) at room temperature has *bcc* structure with a lattice parameter $a = 2.87$ Å. Find the maximum k value of the first Brillouin zone in the $<110>$ direction for iron. (1.5p)

a) See
exam 2008-06-05, problem 3a

b) A Brillouin zone is a primitive cell in the reciprocal lattice, obtained as a Wiegner-Seitz cell construction. Bisect all neighbor distances by planes.

c) Reciprocal lattice of bcc is fcc with side $\frac{4\pi}{a}$



Reciprocal lattice
for Fe.

In <1 1 0> direction, the maximum k is given by the bisected distance between points as in the sketch

This distance is $\frac{1}{4} \cdot \sqrt{2} \cdot \frac{4\pi}{a} = \frac{\sqrt{2}\,\pi}{a}$

4. a) An intrinsic semiconductor has a temperature independent energy gap $\varepsilon_G = 0.8\,\text{eV}$. Assume that the mean free path for electrons and holes are the same at 250 K and 300 K. Estimate the resistivity ratio $\rho(300\,\text{K})/\rho(250\,\text{K})$. State your assumptions. (2p)
b) Explain the following concepts: Indirect bandgap, donor level. (2p)

a) Solution:

$\sigma = n e \mu_e + p e \mu_h$ conductivity, $\rho = \frac{1}{\sigma}$ resistivity

Intrinsic: $n = p = n_i$

Mobility $\mu = \frac{e\tau}{m}$ temp indep. band properties

Mean free path $l = v_F \tau$

$\Rightarrow$ Assume constant mobility

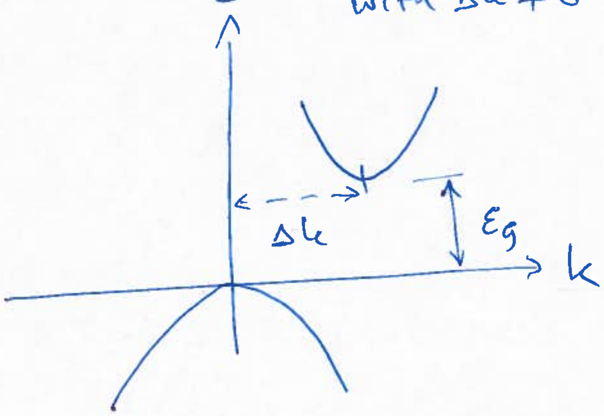
$$\sigma = n_i e (\mu_e + \mu_h)$$

$$\frac{\rho(300)}{\rho(250)} = \frac{n_i(250\text{K})}{n_i(300\text{K})} = \frac{\left(N_c P_v e^{-\mathcal{E}_g/k_BT}\right)^{1/2}\Big|_{250\text{K}}}{\left(N_c P_v e^{-\mathcal{E}_g/k_BT}\right)^{1/2}\Big|_{300\text{K}}} =$$

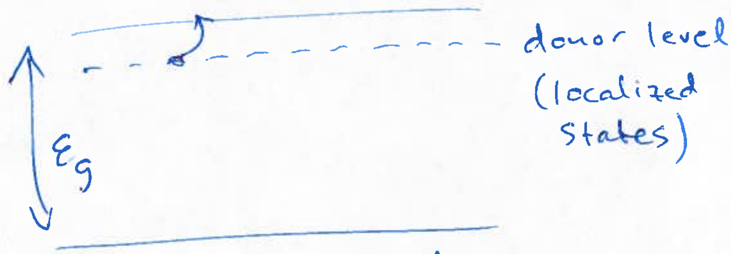
$$= \frac{\left(T^{3/2} e^{-\mathcal{E}_g/2k_BT}\right)\Big|_{250\text{K}}}{\left(T^{3/2} e^{-\mathcal{E}_g/2k_BT}\right)\Big|_{300\text{K}}} = \left(\frac{250}{300}\right)^{3/2} \underbrace{e^{\frac{0.8}{2}\left(\frac{250-300}{300\cdot 250}\right)\cdot\frac{1}{8.62\cdot 10^{-5}}}}_{e^{-3.09}}$$

$$\frac{\rho(300)}{\rho(250)} = 0.034 < 1 \quad \boxed{\text{OK}}$$

b) Indirect bandgap with $\Delta k \neq 0$



Donor level



States in the energy gap that can give away their electrons

5. a) Explain what the Debye model is. (1p)
b) Estimate the Debye temperature for lead (Pb). Lead has a sound velocity $v_s \approx 1190\,\mathrm{m/s}$. (3p)

Solution

a) The Debye model is a model of the phonon $\omega(K)$:

i) $\omega = v_s \cdot |K|$, v_s sound velocity

ii) Cut-off frequency ω_D such that

$$3N = \int_0^{\omega_D} \underbrace{D(\omega)}_{\text{Density of states}}\, d\omega$$

b) Debye temp. Θ_D is defined from

$$\hbar\omega_D = k_B \Theta_D$$

$\Longrightarrow$ Find $\omega_D = v_s \cdot |K|_D$, Find K_D :

$$D(\omega)\,d\omega = D(K)\,dK = \underset{\text{pol dir}}{3} \cdot \underbrace{\left(\frac{L}{2\pi}\right)^3}_{\text{K-vol. per K-point} = \left(\frac{2\pi}{L}\right)^3} \cdot \underbrace{4\pi K^2 dK}_{\text{K-volume}}$$

$$3N = \int_0^{K_D} \frac{3}{2\pi^2} V K^2 dK = \frac{V}{2\pi^2} K_D^3 \; ; \quad \boxed{K_D = \left(6\pi^2 \frac{N}{V}\right)^{1/3}}$$

Pb: fcc structure with $a_{Pb} = 4.95\,\text{Å}$

$$\frac{N}{V} = \frac{4\ \text{at/cell}}{a_{Pb}^3} \Longrightarrow K_D = \left(24\pi^2\right)^{1/3} \cdot \frac{1}{a_{Pb}} = \frac{2\left(3\pi^2\right)^{1/3}}{a_{Pb}}$$

$$\omega_D = 2 \cdot \left(3\pi^2\right)^{1/3} \cdot \frac{v_s}{a_{Pb}} \; ; \quad \Theta_D = 2 \cdot \left(3\pi^2\right)^{1/3} \frac{\hbar v_s}{k_B a_{Pb}}$$

$$\Theta_D = 2 \cdot \left(3\pi^2\right)^{1/3} \cdot \frac{1.055 \cdot 10^{-34} \cdot 1190}{1.38 \cdot 10^{-23} \cdot 4.95 \cdot 10^{-10}} \left[\frac{\cancel{J} \cdot \cancel{s} \cdot \cancel{m}/\cancel{s}}{\frac{\cancel{J}}{K} \cancel{m}}\right] = \underline{\underline{113.7\ K}}$$

(95 K in tables from exp.)

6. a) Pauli paramagnetism is a weak form of paramagnetism, involving itinerant (as opposed to localized) electrons. Make suitable assumptions and deduce an expression for the susceptibility of a Pauli paramagnet. (2p)
b) Discuss two different kind of defects in materials and give examples of their influence on the physical properties. (2p)

a) See exam 2010-03-27, problem 6a

b) See lecture #14

Point defects → resistivity

Dislocations → strength of material

Color centers → optical properties