Solid State Physics

Prof. Dr. Bernd Ploss FH Jena – FB SciTec

Tutorial 1

1. To describe the binding of two atoms i and j one combines an attractive and a repulsive term to form their total interaction energy.

   a) Discuss possible reasons for attractive and repulsive interaction.

   b) Frequently power terms are assumed for the two interactions:

   $$\Phi_{ij}(r_{ij}) = -a/r_{ij}^m + b/r_{ij}^n$$

   Show that a bound state is only possible for $n > m$.

   c) Calculate the static lattice energy U_b of a solid in thermal equilibrium at $T = 0$. Use a cubic unit cell and $r_{ij} = p_{ij} r_1$ with r_1 the distance of next neighbours. Then $r_1^3 = V/(2N_p)$ with N_p the number of atom or ion pairs.

   d) Derive the isothermal compression module $K = -V_0(\mathrm{d}p/\mathrm{d}V)_T$.

   e) In an ionic crystal the Coulomb energy forms the attractive part of the interaction energy. Determine U_b, K, n.

   f) Example NaCl: $\alpha = 1.74$, $K = 3.15 \cdot 10^{10}$ N/m^2, $r_1 = 2.81 \cdot 10^{-10}$ m. How large is the lattice energy per ion pair.

2. Madelung constant α_M

   a) Calculate the Madelung constant for an infinite linear arrangement of positive and negative ions alternating with the distance r_0.

   b) Calculate the Madelung constant for a face centered cubic crystal (NaCl). To get a series which converges fast, the ions should be combined to neutral groups in a smart way.

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Tutorial 2

3. A metal with cubic structure and one atom per lattice point has density 2.6 g/cm^{-3}, molar mass 87.62 g/mol and lattice constant 0.60849 nm. What is the crystal structure of the metal?

4. Indium has a tetragonal structure with $a = 0.3252$ nm and $c = 0.4946$ nm. The density is 7.286 g/cm^{-3} and molar mass 114.82 g/mol. Is the structure simple or body centered tetragonal?

5. What are the Miller indices of a plane through three points with the following coordinates:

   a) (0, 0, 1); (1, 0, 0); (1/2, 1/2, 0)

   b) (1, 0, 0); (0, 0, 1/2); (1/2, 1, 0)

6. The distance d_{hkl} of two parallel net planes (hkl) in a three dimensional orthorhombic system is:

$$d_{hkl}^2 = \frac{1}{(h/a)^2 + (k/b)^2 + (l/c)^2}.$$

   Derive the corresponding equation for the two dimensional case ($l = 0$).

7. a) Derive the equilibrium concentration of point vacancies in a solid which can be described by a minimum of the free energy $F = E - TS$. To obtain the entropy $S = k\ln\Omega$ the number Ω of possible distributions of N_L vacancies over N_G lattice places (i.e. the partition function) must be determined. A useful approximation in this derivation is the Stirling formula $\ln n! \approx n\ln n - n$.

   b) What is the relative concentration of defects N_L/N_G at temperature $T = 1000$ K when the energy to create a vacancy is $E_L = 1$ eV?

c) How precise would one have to measure the density of Si ($\rho = 2.382$ g/cm^{-}3, $A_{\mathrm{rel}} = 28.086$) to prove a density of vacancies of 10^{18} cm^{-3}?

8. a) A face centered cubic lattice is formed by identical atoms. Which is the condition for h, k, l for a reflex not to be extinguished?

b) What is the structure factor F_{hkl} of NaCl? NaCl forms a fcc lattice with a base of one Na^+- and one Cl^--Ion.

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Tutorial 3

9. How high are the sound velocity and the maximum eigenfrequency of iron atoms in a rod which is stimulated to longitudinal vibrations?
   ($E = 2 \cdot 10^{11}$ N/m^2, $a = 2.9 \cdot 10^{-10}$ m, $M = 55.85$ kg/mol, $\rho = 7850$ kg/m^3)

10. Under irradiation of a crystal with laser light of vacuum wavelength $\lambda = 488$ nm Raman radiation is observed at $\lambda = 494$ nm. Waht are the energy and frequency of the generated phonons?

11. Compare momentum and energy of a longitudinal acoustic phonon of wavelength $\lambda = 2.6$ nm and circular frequency $\omega = 8.2 \cdot 10^{13}$ Hz with these of a photon in the green spectral range ($\lambda = 550$ nm).

12. The density of iron is $\rho = 7850$ kg/m^3. How high is the Fermi energy E_F under the assumption that every iron atom allocates one free electron to the crystal? How high is the velocity v_F of electrons with states close to the Fermi level?
    ($M = 55.85$ kg/kmol)

13. The Fermi energy of Na is $E_F = 3.1$ eV. What are the probabilities that the energy levels $E_1 = 3.05$ eV und $E_2 = 3.15$ eV are occupied at temperatures $T = 300$ K and $T = 600$ K, respectively?
    How broad is the transition zone ΔE?

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Tutorial 4

14. How high are mobility μ, relaxation time τ and mean free path l of electrons in copper at room temperature?
    ($\sigma = 5.9 \cdot 10^5\ \Omega^{-1}\mathrm{cm}^{-1}$, $n = 8.5 \cdot 10^{22}\ \mathrm{cm}^{-3}$)

15. Calculate the mean drift velocity of electrons with mobility $\mu = 43\ \mathrm{cm}^2/\mathrm{Vs}$ which are accelerated by a field strength of 100 V/m. Which distance is covered in the direction of the field between two interactions with the crystal lattice at a relaxation time $\tau = 2.5 \cdot 10^{-14}$ s.

16. What is the specific resistance of pure germanium at $T_1 = 300$ K und $T_2 = 200$ K?
    ($n_{i0} = 1.51 \cdot 10^{15}\ \mathrm{cm}^{-3}\mathrm{K}^{-1.5}$, $E_G = 0.66$ eV, $\mu_n(300\ \mathrm{K}) = 3900\ \mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$, $\mu_p(300\ \mathrm{K}) = 1900\ \mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$)

17. Calculate the temperature at which the intrinsic electron concentration of a n-doped silicon sample ($E_G = 1.11$ eV) with a phosphorus donor concentration $n_D = 10^{15}\ \mathrm{cm}^{-3}$ becomes higher than the concentration of the impurities.
    ($n_{i0} = 4.62 \cdot 10^{15}\ \mathrm{cm}^{-3}\mathrm{K}^{-1.5}$)