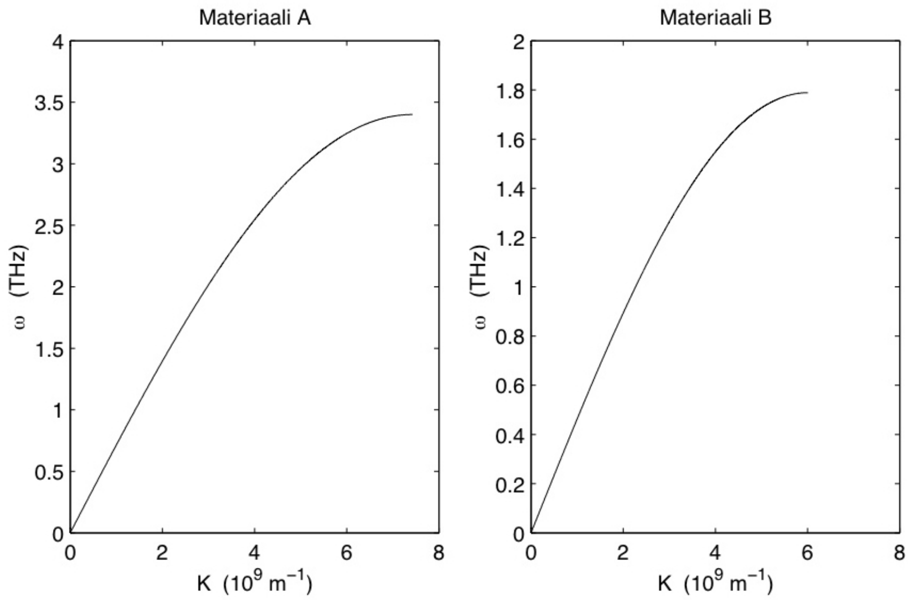
FYSM300 SPRING 2012 INTERMEDIATE EXAM I 8.3.2012

Each problem gives 6 points. Explain your arguments and comment the intermediate steps when you are writing your solutions! Time: 3 hours

1. (a) Argue on the basis of Gibbs free energy that there are always crystal defects present when temperature $T > 0$.
(b) What is a Bravais lattice ?
(c) What is a Schottky pair?
(d) What is a color center?
(e) The figure below shows a dispersion relation $\omega(K)$ for one phonon branch measured for two materials A and B. The materials have the same crystal structure and consist of atoms of the same mass. $\omega(K)$ is shown up to the boundary of the first Brillouin zone. Answer the following: (i) which of the materials has the larger lattice parameter and why? (ii) which of the materials has the higher speed of sound and why?



2. Identify the two different kind of interstitial lattice sites A and B of the FCC structure (face-centered cubic). Calculate the 3D packing fractions of hard spheres for the FCC structure that is
a) fully occupied with atoms at regular lattice sites and at interstitial sites A
b) fully occupied with atoms at regular lattice sites and at interstitial sites B

3. The primitive cell of a certain lattice can be representated with basis vectors $\vec{a}_1 = \frac{\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}$, $\vec{a}_2 = \frac{-\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}$, and $\vec{a}_3 = c\hat{z}$. Calculate the reciprocal lattice for this structure and identify the types of the real space and reciprocal space lattices. What are the lattice constants of the reciprocal lattice? Take the atom basis of $\vec{d_1} = 0$, $\vec{d_2} = \frac{a}{2\sqrt{3}}\hat{x}+\frac{a}{2}\hat{y}+\frac{c}{2}\hat{z}$ for the above mentioned primitive cell and calculate the structure factor $S_{\vec{G}} = \sum_{j,basis} f_j exp(-i\vec{G}\cdot\vec{r}_j)$ by assuming that all the atoms have the same atomic form factor, $f_j = f$.

4. Show by using the Einstein approximation ($= 3N$ harmonic modes, all vibration modes have the same frequency ω_0) that the heat capacity of lattice vibrations can be written as

$$C_v = \frac{\partial}{\partial T}\frac{3N\hbar\omega_0}{e^{\beta\hbar\omega_0} - 1} \tag{1}$$

where $\beta = 1/k_B T$. You can start from the partition function $Z = \sum_i e^{-\beta E_i}$ containing the harmonic vibrational energies or using the information that phonons are bosons. Examine the limiting behaviour of the heat capacity at high and low temperatures. At some point you may want to use the property of the geometric series:

$$s = \sum_{k=0}^{\infty} ar^k = \frac{a}{1-r} \qquad when \quad |r| < 1$$