Advanced Solid State Physics Winter semester 2014/2015 2nd exercise sheet

Submission: Tuesday, 28. October 2014 before the lecture (or drop until 10 o'clock on the same day in mailbox between rooms 1.2.38 and 1.2.40)

4. X-ray scattering at crystal basis containing more than one atom (**) (4 points) In a NaCl crystal Na atoms occupy fcc lattice points, while Cl atoms are sitting mid-way between Na atoms along <100> directions. (Check structure in a book if you are not sure!) Which are the non-vanishing (hkl) X-ray diffraction maxima of NaCl? What can you conclude about their relative intensities?

Use atomic scattering factors f_{Na} und f_{Cl} with $|f_{Na}-f_{Cl}| \ll |f_{Na}+f_{Cl}|$.

5. Two-dimensional diffraction images (**)

Sketch the two-dimensional diffraction images of the following two-dimensional superstructures. Filled and open circles denote different atoms with different atomic scattering factors. Compare your result to the diffraction image of a simple quadratic structure (where filled and open circles are identical atoms).

 $p(2 \times 2)$

p(2×2)	c(2×2)	(3×1)
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6. Recapitulation of introductory solid state physics: Debye model (***) (4 points)

a) Calculate the density of states $g(\omega)d\omega$ of lattice vibrations in a three-dimensional crystal for an isotropic dispersion relation $\omega = vk$.

Hint: $g(\omega)d\omega = g(\mathbf{k})d^3k$ and $g(\mathbf{k}) = \frac{3V}{(2\pi)^3}$ (note that there are three degrees of freedom for vibrations for each k point, one longitudinal and two transversal, thus the factor 3 in the numerator.)

b) Integration of $g(\omega)d\omega$ up to the Debye cut-off frequency ω_D yields 3N, three times the number of atoms.

Estimate the Debye temperature Θ_D for an atom density $N/V = 4/(3.61 \text{ Å})^3$ and v = 3000 m/s.

(4 points)