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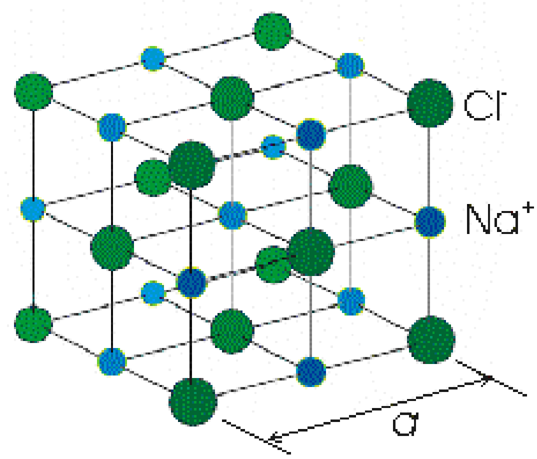
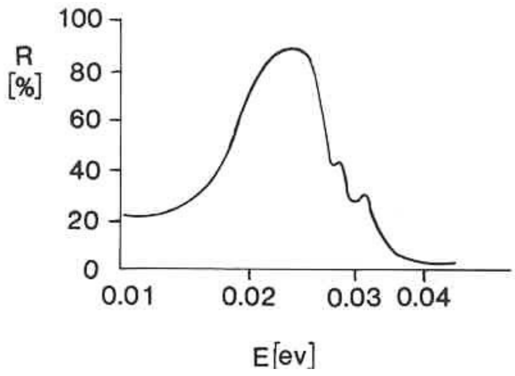
Exercises "Advanced materials B"

6

Exercise 6: Ionic polarization



(a)



(b)

Fig. 1: (a) NaCl crystal structure. **(b)** Optical reflection spectra of NaCl in the far IR regime.

a) Discuss shortly the three major types of bonds in a crystal.
b) Explain qualitatively how ionic polarization works. What are the opposing forces? What is the connection to phonons?
c) How do lattice atoms move when an acoustic, respectively optical phonon is excited? Which type of phonon can thus only be responsible for ionic polarization?
d) Calculate the spring constant k for NaCl (**Fig. 1(a)**, Young's modulus Y_{NaCl} = 40.0 GPa, lattice constant a_{NaCl} = 0.58 nm).
The angular resonance frequency ω_0 of this diatomic system is given by $\omega_0^2 = 2k\left(\frac{1}{m_{\mathrm{Na}}} + \frac{1}{m_{\mathrm{Cl}}}\right)$.
e) Calculate the actual resonance frequency ω_0 (M_{Na} = 23.0 g/mol, M_{Cl} = 35.5 g/mol).
f) Determine the equilibrium distance d_E for an electrical field E = 100 kV/cm.

Fig. 1(b) shows the optical reflectance of NaCl in the far infrared (FIR).
g) How are transmission T, absorption A, and reflection R connected?
h) Is a peak in the reflection an automatical sign of a resonance in the dielectric function $\varepsilon(\omega)$?

Assume for the rest that the reflection peak in **Fig. 1(b)** is indeed caused by a resonance phenomenon, i.e. the electromagnetic wave used for the reflection measurement induces a phonon, which later re-emits an electromagnetic wave.
i) Determine the wavelength λ and frequency f of the electromagnetic wave at the major reflection peak at 25 meV. Compare these values with your theoretically calculated values for the phonon (see **(e)**).