

Each problem gives 6 points. Time limit 3h.

1. Explain shortly

- a) crystal structure
- b) fractals
- c) Schottky pair
- d) color center
- e) van der Waals interaction
- f) Arrhenius behavior

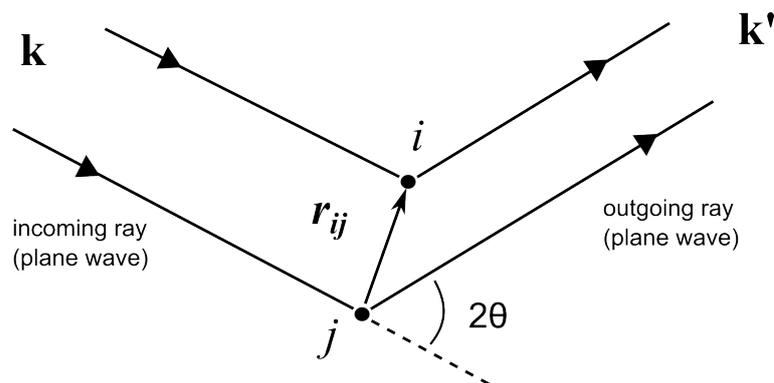
2. One specific real-space lattice can be described by primitive vectors $\mathbf{a}_1 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$, $\mathbf{a}_2 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$ and $\mathbf{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$, where a is a lattice parameter.

- a) Draw and identify the lattice.
- b) Determine the coordination number and the nearest neighbour distance for this lattice.
- c) Calculate packing fraction $\eta = \frac{V_{\text{spheres}}}{V_{\text{unit cell}}}$ of this lattice.
- d) Determine, draw and identify the reciprocal space lattice and the corresponding reciprocal space lattice parameter.

Take (110) plane of the 3D real-space lattice that was defined above and consider the plane to be a separate 2D-lattice. For this lattice draw and define

- e) primitive vectors
- f) Wigner-Seitz cell

3. Using the figure below (i and j are lattice points), derive the Laue condition of diffraction from crystal structure by elastic scattering. In other words show that $\mathbf{K} = \mathbf{G}$, where $\mathbf{K} = \mathbf{k}' - \mathbf{k}$ is the scattering vector, \mathbf{k} and \mathbf{k}' are the wavevectors of the incoming and outgoing plane waves and \mathbf{G} is the reciprocal lattice vector of the crystal. Explain the intermediate steps in detail and if necessary draw figures! What is the meaning and interpretation of the Bragg planes and the structure factor to the diffraction from crystal structures?



4. a) Derive the dispersion relation $\omega(k)$ for the atomic dynamics in a periodic 1D chain with identical atom masses M connected with identical springs (spring constant K). Include only (harmonic) nearest neighbour interactions. Sketch the dispersion curve and mark the Brillouin zone

edges. What are the group velocities at the Brillouin zone edge and at the Brillouin zone center? Identify the type of the phonon branch (acoustic or optic). Explain qualitatively how the dispersion relation would change if the interactions beyond nearest neighbours would be included.

b) Determine the heat capacity of one simple harmonic oscillator. Start by writing the internal energy of the system (namely the thermal average of the total energy). Why the energy of the system is not zero at $T=0$?

$$\exp(ix) = \cos(x) + i \sin(x)$$

$$a + ar + ar^2 + ar^3 + \dots = \frac{a}{1-r}$$