

Frankfurt, Oct. 21, 2009

Theoretikum zur Einführung in die Theoretische Festkörperphysik
WS 2009/10

Exercise Set 1

(Due date: Tuesday, Oct. 27, 2009)

Exercise 1 (Bravais lattice) (10 points)

A Bravais lattice $\vec{R} \equiv \vec{R}_{\vec{n}}$ is given.

- Show that the reciprocal lattice, defined by $e^{i\vec{k}\cdot\vec{R}} = 1$ is also a Bravais lattice.
- Show that fcc and bcc lattices are mutually reciprocal. Show for this case that volume of the unit cell of the reciprocal lattice is inversely proportional to the volume of the unit cell of the Bravais lattice.

Exercise 2 (Centered rectangular lattice) (10 points)

- Determine the reciprocal lattice of a centered rectangular lattice. Which Bravais lattice do you get?
- Draw the first Brillouin zone of the centered rectangular lattice.

Exercise 3 (Crystal structure of La_2CuO_4) (15 points)

La_2CuO_4 has a tetragonal body centered structure with the atoms arranged in the conventional unit cell (with a square face of $\mathbf{a}_1 = \mathbf{a}_2 = \mathbf{a} \approx 3.8 \text{ \AA}$ and $\mathbf{a}_3 = \mathbf{c} \approx 13.2 \text{ \AA}$) as follows:

Cu at $(0, 0, 0)$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

O at $(\frac{1}{2}, 0, 0)$, $(0, \frac{1}{2}, 0)$, $(0, 0, \frac{1}{6})$, $(\frac{1}{2}, \frac{1}{2}, \frac{1}{3})$, $(1, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 1, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, \frac{2}{3})$, $(1, 1, \frac{5}{6})$.

La at $(0, 0, \frac{1}{3})$, $(\frac{1}{2}, \frac{1}{2}, \frac{1}{6})$, $(\frac{1}{2}, \frac{1}{2}, \frac{5}{6})$, $(1, 1, \frac{2}{3})$.

- Sketch this structure by drawing the atom distribution in one (to four) conventional unit cells.
- How many formula units do you have per conventional and per primitive unit cell?

- c) Convince yourself that each copper ion is surrounded by an octahedron of six oxygen ions (which is slightly stretched in c direction).
- d) Convince yourself that at a distance of $c/2$, CuO_2 layers are formed, and determine the lattice and basis of these two dimensional layers.