Problem set 2

Problem 1 Face-Centered Cubic and Body-Centered Cubic lattices

In the lecture we briefly discussed the face-centered cubic (FCC) and body-centered cubic (BCC) lattices. In this problem, we want to understand their properties in a bit more detail, assuming a single-atom basis.

(1.a) Assume that a solid is made of hard spheres that are touching each other. Find the volume fraction occupied by the spheres for the BCC and FCC latices.

(1.b) The coordination number is defined as the number of nearest neighboring lattice sites. Find the coordination numbers for the FCC and BCC lattice and deduce the number of atoms per unit cell.

(1.c) Show that the three primitive vectors of the FCC lattice span a regular tetrahedron.

(1.d) Show that the reciprocal lattice of an FCC lattice is a BCC lattice, and vice versa. Determine the corresponding lattice constants of the reciprocal lattices in terms of those of the direct lattice.

Problem 2 Graphene and friends

In general, we are faced with the situation that the atomic basis at each Bravais lattice point contains more than one atom. Here, we investigate this situation at the example of graphene and hexagonal boron nitride, which come with a two-atomic basis.

(2.a) Show that the honeycomb lattice is not a Bravais lattice and that, instead, it can be considered as a bipartite lattice structure with a two-atomic basis (which we denote by type A and B). Find the underlying Bravais lattice and the atomic basis vectors.

(2.b) Show that graphene, whose carbon atoms can be placed at the corners of a honeycomb lattice, has one six-fold, two three-fold and three two-fold rotation axis. Hexagonal boron nitride comes with two different species of atoms forming a honeycomb lattice. The A-type sites can be considered to be occupied by boron and the B-type sites can be considered to be occupied by nitrogen atoms. What happens to the rotational symmetries in that case?

(2.c) Construct the reciprocal lattice of the honeycomb lattice.

Problem 3 Five is impossible

Show that there can be no five-fold rotation axis in a Bravais lattice. You may use the fact that certain rotations around an angle ϑ, denoted by the matrix $\mathbf{R}(\vartheta)$, map Bravais lattice points into each other.

Problem 4 A lattice is a lattice is a lattice: Equivalent Bravais lattice definitions

In the lecture we mentioned that the following two definitions of a Bravais lattice are equivalent

1. A Bravais lattice is a set of points of the form $\vec{R}_{\vec{n}} = n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3$, where $\vec{n} = (n_1, n_2, n_3)$ is a triple of integers (of any sign) and the vectors $\vec{a}_j,\ j = 1, 2, 3$ are the primitive lattice vectors.

2. A Bravais lattice is closed under addition and subtraction: if $\vec{R}_{\vec{n}}$ and $\vec{R}_{\vec{m}}$ are elements of the lattice, then $\vec{R}_{\vec{n}+\vec{m}} = \vec{R}_{\vec{n}} \pm \vec{R}_{\vec{m}}$ is also an element of the lattice.