Exercise 1 - Crystal Structure

(3 points)

(a) The primitive vectors for a body center cubic (bcc) lattice are

$$\vec{a}_1 = a\vec{x},$$

 $\vec{a}_2 = a\vec{y},$
 $\vec{a}_3 = \frac{a}{2}(\vec{x} + \vec{y} + \vec{z}).$

or, in a more symmetric set

$$\vec{a}_1 = \frac{a}{2}(-\vec{x} + \vec{y} + \vec{z}),$$

$$\vec{a}_2 = \frac{a}{2}(\vec{x} - \vec{y} + \vec{z}),$$

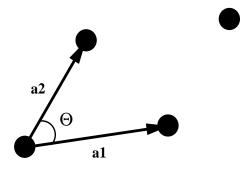
$$\vec{a}_3 = \frac{a}{2}(\vec{x} + \vec{y} - \vec{z}).$$

- 1. Make a drawing of this lattice,
- 2. Find the reciprocal lattice vectors and make a drawing of the reciprocal lattice.
- (b) The primitive vectors for a face center cubic (fcc) lattice are

$$\vec{a}_1 = \frac{a}{2}(\vec{y} + \vec{z}),$$

 $\vec{a}_2 = \frac{a}{2}(\vec{x} + \vec{z}),$
 $\vec{a}_3 = \frac{a}{2}(\vec{x} + \vec{y}).$

- 1. Make a drawing of this lattice,
- 2. Find the reciprocal lattice vectors and make a drawing of the reciprocal lattice.
- (c) Graphically construct the Wigner-Seitz cell and the reciprocal lattice of the two dimensional oblique lattice with basis vectors $\vec{a}1$ and $\vec{a}2$ shown in the following sketch:



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SS 2013 Sheet 1

Prof. Dr. A. Muramatsu

Exercise 2 - The Brillouin Zone

(1 points)

Show that the volume of the elementary cell Ω and the volume of the Brillouin Zone Ω_B are connected by the following relation:

$$\Omega_B = \frac{(2\pi)^3}{\Omega} \tag{1}$$

Exercise 3 - Tetragonal symmetry

(2 points)

Show that if one streches a fcc lattice along one of its lattice vectors, the resulting lattice is equivalent to a tetragonal body centered lattice. So the point group with the tetragonal symmetry has two Bravais lattices: simple tetragonal and body centered tetragonal, whereas the point group with cubic symmetry has three Bravais lattices: sc, bcc and fcc.

Exercise 4 - Fourier transformations

(2 points)

- 1. Calculate the Fourier coefficients for a function f(x) = c, c some number, x defined in some one-dimensional interval.
- 2. Calculate explicitly the Fourier coefficients for a function $f(x) = \exp(i p \frac{2\pi}{a} x)$, with p some integer.

Solutions due on the 15th of April, 2013