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Exercise Set 2

(Due date: Tuesday, November. 3, 2009)

Exercise 4 (**Reciprocal lattice and Brillouin zone**) (10 points)

The basis vectors of a primitive monoclinic unit cell are given in Cartesian coordinates as

$$\vec{a}_1 = \vec{e}_x - \vec{e}_y$$
$$\vec{a}_2 = 2\vec{e}_x + \vec{e}_y$$
$$\vec{a}_3 = \frac{1}{2}\vec{e}_z$$

a) Determine the reciprocal lattice and explain its relation to Bragg reflections.

b) Draw the first Brillouin zone.

Exercise 5 (**Bragg's law**) (5 points)

A beam of electrons with kinetic energy 1 keV is diffracted when passing through a metal. The metal has a cubic structure with lattice parameter $a = 1$ Å. Please find the necessary constants in any quantum physics book.

a) Calculate the wavelength of the electrons.

b) Calculate the Bragg angle for the first order diffraction maximum.

Exercise 6 (**Orthonormality on the reciprocal lattice**) (15 points)

Prove the two relations

a) $$\frac{V_{\mathrm{puc}}}{(2\pi)^3}\int_{1\mathrm{st\,BZ}} d^3k\, e^{i\vec{k}\cdot(\vec{R}-\vec{R}')} = \delta_{\vec{R},\vec{R}'}$$

b) $$\frac{V_{\mathrm{puc}}}{(2\pi)^3}\sum_{\vec{R}\in R} e^{i\vec{k}\cdot\vec{R}} = \sum_{\vec{G}\in R^*}\delta\left(\vec{k}-\vec{G}\right)$$

where V_{puc} is the volume of the primitive unit cell, and R and R^* are direct and reciprocal lattices, respectively.