5   Surfaces, Interfaces, Diffraction

5.1   **Determine the energies of X-ray photons and electrons with the wavelength of 0.1 nm = 1 $\dot{A}$. Using these energies, please discuss the conclusions from the BRAGG equation considering the lattice spacing of 1.8 $\dot{A}$ (example Ni(100)).**

Given that:
λ =0.1 nm=0.1 $\cdot 10^{-9}$ m=1 $\dot{A}$ - wavelength of photons and electrons;
$h = 6.62620 \cdot 10^{-34}$ J $\cdot$ s - Planck's constant;
$c = 2.9979 \cdot 10^{8}$ m/s - speed of light in a vacuum;
$m = 9.10956 \cdot 10^{-31}$ g - mass of electron;
$d = 1.8$ $\dot{A}$ - lattice spacing.

(a) The energies of X-ray photons:
$E = h \cdot \nu = (h \cdot c)/\lambda = 1.9846 \cdot 10^{-15}$ J=12.3867 keV.

(b) The energies of electrons:
$E = h^2/(2 \cdot m \cdot \lambda^2) = 2.4099 \cdot 10^{-17}$ J=0.1504 keV.

(c) Bragg equation:
$2 \cdot d \cdot sin\theta = n \cdot \lambda$
Constructive interference occurs when the path difference is an integral number n of the wavelength. Note that the equation can only be fulfilled, if the wavelength is smaller than 2 lattice spacings d. So,
$sin\theta = (n \cdot \lambda)/(2 \cdot d)$;
$-1 \leq sin\theta \leq 1$;
$\Rightarrow -1 \leq (n \cdot \lambda)/(2 \cdot d) \leq 1$;
$\Rightarrow -1 \leq \frac{5}{18}n \leq 1$;
$\Rightarrow -3.6 \leq n \leq 3.6$. n is integer $\Rightarrow$ n= $\pm3; \pm2; \pm1; 0$
$\Rightarrow \theta = 0^0, \pm16.1^0, \pm33.6^0, \pm56.4^0$.

5.2 In an ideal gas at room temperature, the density of particles (atoms and molecules) and their mean free path should be estimated for atmospheric pressure ($10^5 Pa$) and vacua of $10^{-4}, 10^{-6}$, $10^{-8}, 10^{-10} Pa$ (use simple equations of kinetic gas theory). Demonstrate the necessity of vacuum conditions for surface studies by estimating the time for the formation of one monolayer using the pressures given above assuming that all particles (atoms or molecules) will be absorbed and not be re-evaporated.

An **ideal gas** is a gas composed of a set of non-interacting point particles.

Room temperature is a general term describing common indoor temperatures. For numerical convenience, either 20 °C or 300 K is often used.

(a) Atmospheric pressure

$p = 10^5$ Pa - atmospheric pressure;
$T = 20$ °C $= 293$ K - temperature;
$V = 1$ cm^3 - volume;
$k = 1.380648812 \cdot 10^{-23}$ J$\cdot$ K^{-1} - Boltzmann constant;
$m_N = 14$ g/mol - molar mass of nitrogen;
$m_{N_2} = 28$ g/mol - molar mass of N_2;
$N = \frac{PV}{kT}$ - The equation of state of an ideal gas;
$N_m = \frac{PV}{kT} = 2.5 \cdot 10^{19}$ - number of molecules of at room temperature in atmospheric pressure within $1 cm^3$;
$N_a = N_m \cdot 2 = 5 \cdot 10^{19}$ - number of atoms;
$\rho_m = N_m/V = 2.5 \cdot 10^{19}$ N/cm^3 - density of particles (molecules);
$\rho_a = N_a/V = 5 \cdot 10^{19}$ N/cm^3 - density of particles (atoms);
$d = 120 \cdot 10^{-12}$ m - diameter of the gas particles (ideal gas particle does not have any size.)
$\lambda = \frac{kT}{\sqrt{2}\pi d^2 P} = 6.323 \cdot 10^{-8}$ m - mean free path;
$\frac{dN}{dA \cdot dt} = \frac{p}{\sqrt{2\pi \cdot mkT}} = 1.109 \cdot 10^{15}$ /m$^2\cdot$ s $\Rightarrow t = 3$ ns ;

(b) $p = 10^{-4}$ Pa
$\rho = N/V = 2.5 \cdot 10^{10}$ N/cm^3 - density of particles (molecules);
$\lambda = \frac{kT}{\sqrt{2}\pi d^2 p} = 60$ m- mean free path;
time for ML formation t=3 s.

(c) $p = 10^{-6} Pa$

$\rho = N/V = 2.472 \cdot 10^8 N/cm^3$ - density of particles (molecules);
$l = \frac{kT}{\sqrt{2}\pi d^2 p} = 6.323$ km- mean free path;
time for ML formation t=5 min.

(d) $p = 10^{-8} Pa$
$\rho = N/V = 2.472 \cdot 10^6 N/cm^3$ - density of particles (molecules);
$l = \frac{kT}{\sqrt{2}\pi d^2 p} = 632.3$ km- mean free path;
time for ML formation t=8.5 h.

(e) $p = 10^{-10} Pa$
$\rho = N/V = 2.472 \cdot 10^4 N/cm^3$ - density of particles (molecules);
$l = \frac{kT}{\sqrt{2}\pi d^2 p} = 63233$ km - mean free path;
time for ML formation t=35 d.

5.3 **Please draw the surface unit cell termed $(\sqrt{3} \times \sqrt{3})\mathbf{R}\ 30^0$ for Si(111). This reconstruction occurs in boron-doped Si(111) after heating to 1200 °C because of boron segregation under ultra-high vacuum conditions. Describe the changes of the electron diffraction pattern during this phase transition, qualitatively.**
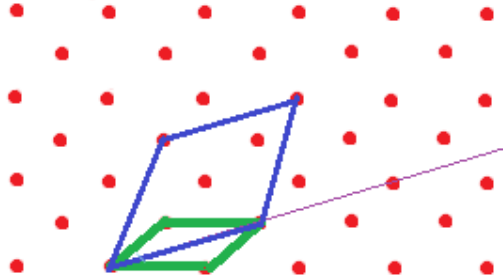

Figure 1: The surface unit cell: (1×1) - green colored; $(\sqrt{3} \times \sqrt{3})$R 30^0 - blue colored

The Si (111) surface has 6-fold symmetry.
The green-colored unit cell is the unreconstructed cell. Its sides are defined to be 1 unit long. The 3 times larger blue-colored unit cell is the $\sqrt{3}$ structure.
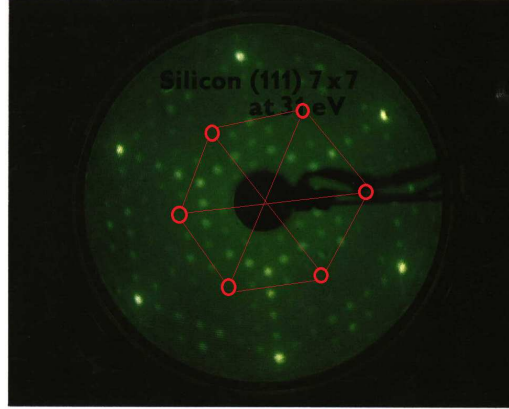
Figure 2: Silicon (111) 7x7 at 31eV.

The diffraction image of the Si (111)- $(\sqrt{3} \times \sqrt{3})$R 30^0 has additional spots as indicated in Figure 4 by the red-colored circles.

5.4 A calculation should demonstrate that the reciprocal lattice to the fcc lattice is the bcc lattice and vice versa.

(a) **Reciprocal lattice to bcc structure**

The primitive translation vectors of the bcc lattice are:

$$a_1 = \tfrac{1}{2}(-\hat{x} + \hat{y} + \hat{z}); \; a_2 = \tfrac{1}{2}(\hat{x} - \hat{y} + \hat{z}); \; a_3 = \tfrac{1}{2}(\hat{x} + \hat{y} - \hat{z}).$$

Here a is the side of the conventional cube and x, y, z are orthogonal unit vectors parallel to the cube edges.

The primitive translations of the reciprocal lattice are defined as:

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3}; \; b_2 = 2\pi \frac{a_3 \times a_1}{a_1 \cdot a_2 \times a_3}; \; b_1 = 2\pi \frac{a_1 \times a_2}{a_1 \cdot a_2 \times a_3}.$$

So now we have:

$$b_1 = (2\pi/a)(\hat{y} + \hat{z}); \; b_2 = (2\pi/a)(\hat{x} + \hat{z}); \; b_3 = (2\pi/a)(\hat{x} + \hat{y}).$$

These are just the primitive vectors of an fcc lattice, so that an fcc lattice is the reciprocal lattice of the bcc lattice.

4

(b) Reciprocal Lattice to fcc structure

The primitive translation vectors of the fcc lattice are:

$$a_1 = \tfrac{1}{2}(\hat{y} + \hat{z}); \; a_2 = \tfrac{1}{2}(\hat{x} + \hat{z}); \; a_3 = \tfrac{1}{2}(\hat{x} + \hat{y}).$$

The primitive translation vectors of the lattice reciprocal to the bcc lattice are:

$$b_1 = (2\pi/a)(-\hat{x} + \hat{y} + \hat{z}); \; b_2 = (2\pi/a)(\hat{x} - \hat{y} + \hat{z}); \; b_3 = (2\pi/a)(\hat{x} + \hat{y} - \hat{z}).$$

These are primitive translation vectors of a bcc lattice, so that the bcc lattice is reciprocal to the fcc lattice.