Problem Set – Elastic x-ray scattering

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PHY585: Principles of Non-Relativistic Scattering Applications, Block Course

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Note: to make your lives a little easier, those powerpoint slides from this part of the course that are most relevant to solving this problem set are flagged top-right with the image:

1 Hints

- A practical expression relating photon energy to its wavelength is $\lambda[\text{Å}] = 12.3984/E[\text{keV}]$
- A scattering vector Q or wavevector k in reciprocal space of magnitude G corresponds to a distance (or wavelength) in real space of $2\pi/G$.
- The volume of a sphere of radius r is $(4\pi/3)r^3$.
- $\exp(iX\pi)$ for $X > 2 = \exp(i[X \bmod 2]\pi)$, whereby $X \bmod 2$ is the remainder of $X/2$.
- The triangle formed by the incoming and outgoing wavevectors of magnitude k and the scattering vector Q in elastic scattering of radiation with wavevector k is isosceles, with a vertex angle equal to 2θ and a base length equal to the scattering vector Q.

2 Problems

Problem 1.1. The so-called 'Poynting vector', S, defines the energy flow per unit area and unit time of electromagnetic radiation and is given by

$$S = \frac{\epsilon_0 E_0^2 c}{2},$$

whereby E_0 is the amplitude of the electric-field component, $\epsilon_0 = 8.854 \times 10^{-12}$ As/Vm is the permittivity of free space and $c = 2.9979 \times 10^8$ m/s is the speed of light. Determine the electric-field amplitude E_0 for an x-ray beam consisting of 10^{14} 10-keV photon/s and a top-hat profile of 0.01 mm^2. What is the amplitude of the associated oscillatory electric force acting on an electron, expressed in fN (10^{-15} N)?

Problem 1.2. A diffraction experiment runs at a photon energy of 12.658 keV. What is the volume of the Ewald sphere in cubic reciprocal Angstroms? How many Bragg peaks lie within the bounds of the Ewald sphere for a tetragonal crystal with lattice constants $a = b = 7$ Å and $c = 3.9$ Å?

Problem 1.3. A powder diffraction pattern of an orthorhombic crystal is recorded. The following data was extracted:

- (1 0 1) peak at 1.128008 Å^{-1},
- (2 0 0) peak at 1.414758 Å^{-1},
- (0 1 1) peak at 1.449354 Å^{-1}.

The equation to determine interplanar spacings, $d_{(hkl)}$, for orthorhombic crystals is given by

$$d^2_{(hkl)} = \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right)^{-1}.$$

Using this information, determine the unit-cell volume in Å^3.

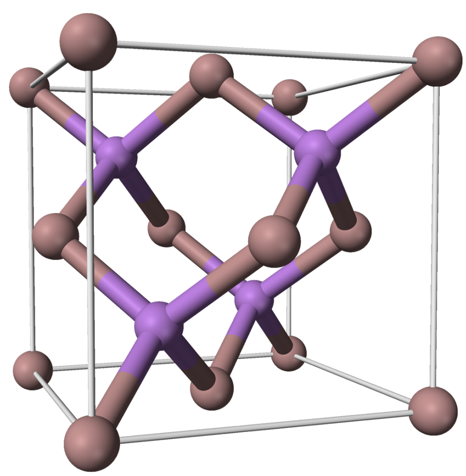

Figure 1: The unit cell of face-centered cubic GaAs. The unit cell is composed of four Ga-atoms at $(0,0,0)$, $(0,1/2,1/2)$, $(1/2,0,1/2)$, and $(1/2,1/2,0)$; and four As-atoms at $(1/4,1/4,1/4)$, $(1/4,3/4,3/4)$, $(3/4,1/4,3/4)$, and $(3/4,3/4,1/4)$, in units of the lattice constant.

Problem 1.4. Consider the unit-cell configuration of GaAs in Figure 1. Demonstrate that the expression for the structure factor F of the (311) Bragg peak of GaAs is

$$F = 4(f_{Ga} - i f_{As}),$$

whereby f_{Ga} and f_{As} are the atomic form factors for Ga and As, respectively.

Problem 1.5. This question addresses the overlap problem associated with Laue diffraction. Figure 2 is a (not to scale) schematic of a Laue diffraction setup. The h-axis points antiparallel to the incident radiation, and the l-axis points vertically, as shown. Also shown is the line trace that passes through the $m(102)$ Bragg

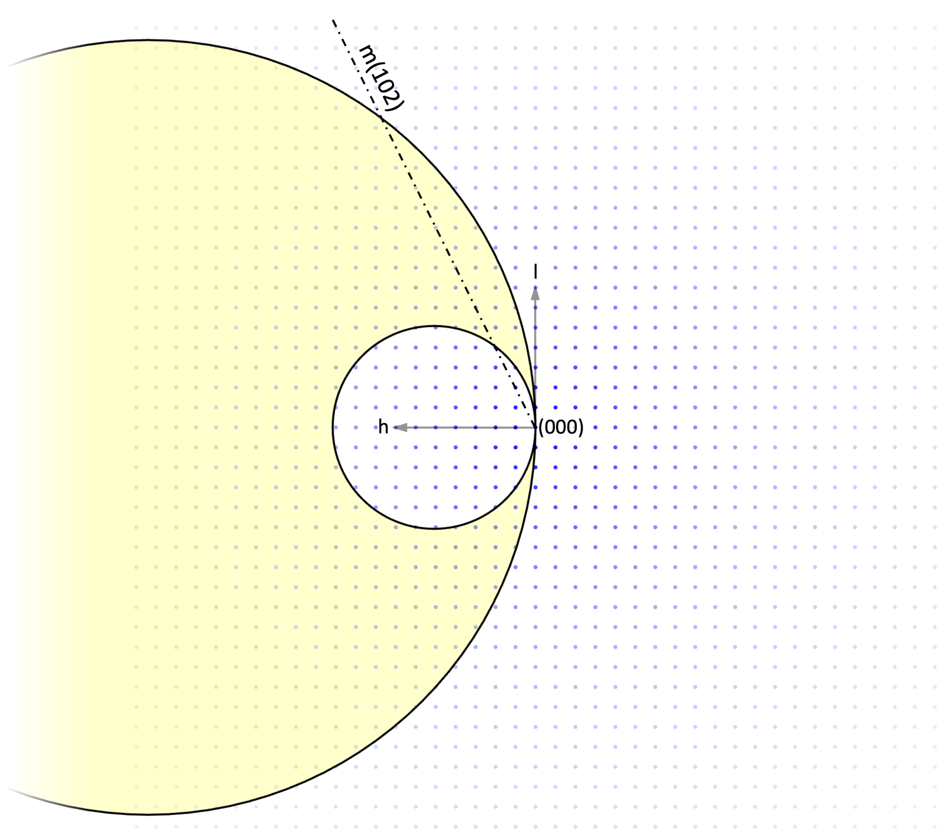

Figure 2: A not-to-scale schematic of a crystal diffraction pattern and the Laue volume associated with a broadband radiation of 5 to 20 keV. The dashed line passes through the set of $m(102)$ Bragg peaks.

reflections [that is, the (102), (204), (306)...etc. reflections] - these will all overlap with one another, as their scattering directions are identical.

The crystal generating this pattern has a primitive cubic unit cell with a lattice constant $a = 100$ Å. The polychromatic radiation spans 5 to 20 keV. What are the minimum and maximum values of m that are simultaneously recorded?

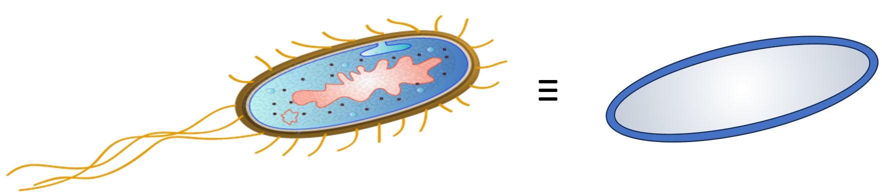

Figure 3: The bacterium *Escherichia coli* can be well approximated as a hollow prolate ellipsoid.

Problem 1.6. The bacterium *Escherichia coli* can, in terms of SAXS experiments, be approximated as being a hollow prolate ellipsoid (cigar shaped) with a length of 1 μm, largest girth diameter of 0.5 μm, and a wall thickness of 40 nm (see Figure 3). Calculate its radius of gyration R_G in nm. Refer to the table provided in the powerpoint presentation "Scatt2v2.pptx".