Physics with neutrons 1

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Winter semester 2015/16
Exercise sheet 8
Due 2015–Dec–11

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Exercise 8.1

Diffraction of neutrons from argon monolayers absorbed on graphite basal planes indicated that an ordered, two dimensional triangular argon lattice is formed at low temperatures [Taub et. al. (1977)], see Fig. 1. There are two possible configurations for the argon monolayers, either commensurate with the graphite lattice or incommensurate corresponding to the closest packing.
(a) Explain the asymmetric sawtooth profile of the Bragg peaks in Fig. 1.
(b) Determine from the observed reflections displayed in Fig. 1 whether the Ar monolayers are commensurate or incommensurate with the graphite lattice. The C atoms have a nearest neighbor distance $a_C = 2.46$ Å in the hexagonal plane of graphite.

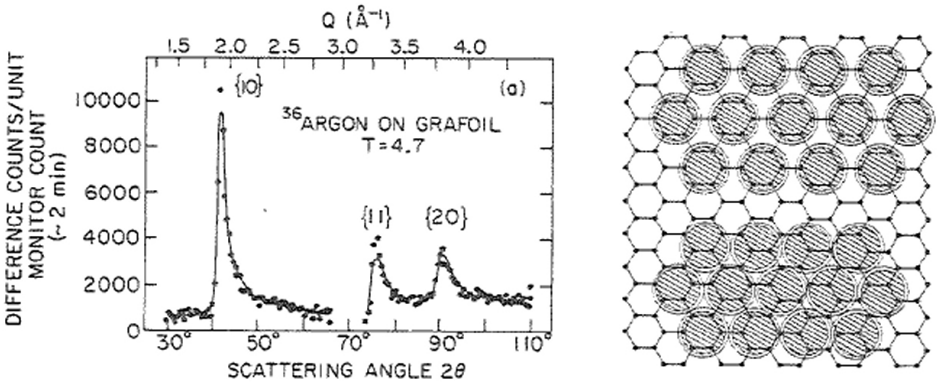

Figure 1: (left) Diffraction pattern from a two-dimensional Ar monolayer absorbed on graphite showing the Bragg reflections (1,0), (1,1) and (2,0). (right) Schematic representation of a commensurate (top) and incommensurate (bottom) Ar monolayer phase.

Solution. a) The reciprocal lattice of a two-dimensional crystal consists of an ordered array of rods aligned normal to the scattering plane. In diffraction experiments there is for each Miller index pair (h, k) a minimum value of the scattering angle $2\theta = 2\theta_B$ where θ_B corresponds to the Bragg angle

$$\lambda = 2d \sin\theta_B. \tag{1}$$

Depending on the size of the array, there will be a continuous distribution of diffracted intensity for scattering angles greater than $2\theta_B$. This produces a characteristic *sawtooth* line shape with a sharply rising leading edge on the low-angle side, followed by a trailing edge extending to larger scattering angles. The maximum of the diffracted intensity I_{hk} occurs at the scattering angle $2\theta_B$. For a detailed calculation of the line shape we refer to the basic article by Warren [Warren (1941)]:

$$I_{hk} = \frac{m_{hk}|S_{hk}|^2 L(\theta)}{\sin\theta\sqrt{\sin^2\theta - \sin^2\theta_B}},$$

where m_{hk} denotes the multiplicity of the Bragg reflection (h,k,l), $L(\theta)$ is the Lorentz factor.

b) Following EXERCISE 5.2, the reciprocal lattice vectors of a two-dimensional heagonal lattice are given

$$\tau_1 = \frac{2\pi a}{f_0}(\sqrt{3}/2, 1/2), \tau_2 = \frac{2\pi a}{f_0}(0,1), f_0 = \frac{\sqrt{3}}{2}a^2,$$

where a is the nearest-neighbor distance. By identifying the peaks observed at $Q = 1.9, 3.3$ and 3.8 Å^{-1} as the $(1,0), (1,1)$ and $(2,0)$ Bragg reflections, we find from Eq. (1) $a_{\mathrm{Ar}} = 3.82$ Å. This is significantly smaller than the distance $\sqrt{3}a_C = 4.26$ Åfor the commensurate phase sketched in Fig 1, thus the Ar monolayer is clearly incommensurate with that of the underlying graphite basal plane. $a_{\mathrm{Ar}} = 3.82$ Åcorresponds to the minimum of the Lennard-Jones potential $\Phi(r) = -Ar^{-6} + Br^{-12}$ known for solid Ar. We conclude that the structure of the Ar monolayer is primarily determined by the couplings between the Ar atoms, and interactions with the substrate appear to play a minor role.

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EXERCISE 8.2

Practicals on powder diffraction data with the program Fullprof.

EXERCISE 8.3

Practical on SANS data with the program SASFit.