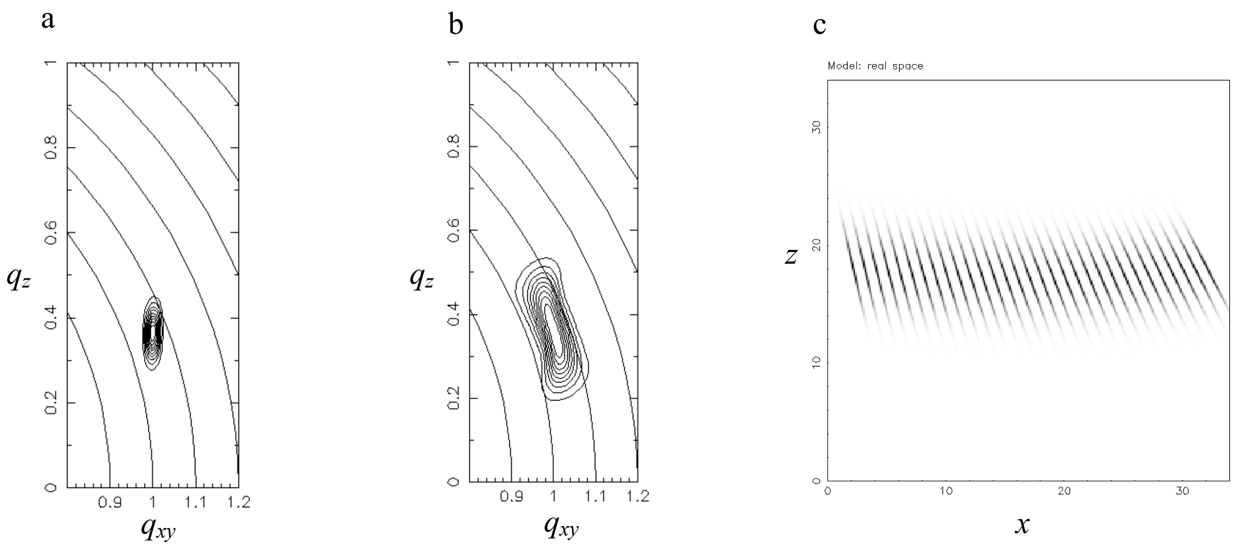
2.6.1 X-ray Diffraction from Curved Thin Films

P. B. Howes, K. Kjær, *Risø National Laboratory, DK4000 Roskilde, Denmark.*

X-ray diffraction has proved to be a powerful technique in the study of Langmuir monolayers. It is well known that diffraction from a flat, two-dimensional, crystalline monolayer leads to rods of scattering in reciprocal space which are sharp in the directions parallel to the surface, $\boldsymbol{q}_{xy}$, but extended perpendicular to the surface: along $\boldsymbol{q}_z$. A number of experiments on amphiphilic mono- or multi-layers have given rise to diffraction which, instead of exhibiting the expected Bragg rod (see Fig. 1a), are additionally extended along a curved line[1] which follows the Scherrer ring of constant $(q_{xy}^2 + q_z^2)^{1/2}$ (see Fig. 1b). Such scattering can be explained by a mosaic spread in the normals of flat crystallites[2]. Another possible explanation is that the individual crystallites may be curved (Fig 1c); however it is not immediately obvious if this would give rise to the observed peak profile, or whether an X-ray diffraction experiment could distinguish the two cases. To investigate this phenomenon, we have performed numerical simulations of the X-ray scattering from both curved crystallites and mosaic distributions of flat crystallites. The simulations were performed on one-dimensional crystals (Fig 1c). The electron density of the long, linear molecules was taken to be a Gaussian ellipse for simplicity. For the curved domains, the scattered intensity was calculated as the coherent sum in reciprocal space of the Fourier transforms of N molecules on a circularly curved line with radius R. For the case of a mosaic spread of flat crystallites the Fourier transform of the density of a single crystallite was first calculated then added incoherently to that from other crystallites with different tilts.

It was found that the two different kinds of surface gave broadly similar scattering. In both cases the Bragg rod was extended along the Scherrer ring (Fig 1b). However, whereas the mosaic crystallites lead to a constant q_{xy}-width, the curved layer diffraction becomes broader with increasing diffraction order. Thus it is, in principle, possible to distinguish the two cases experimentally.

Fig. 1. Calculated diffraction peak profiles for a flat monolayer (N=30) (a) and a curved monolayer (N=30, R=120 intermolecular spacings) (b). Real space electron density of the curved monolayer is shown in (c).



[1] S. P. Weinbach *et al.,* Ann. Rep. Solid State Physics Dept., Risø, 1994, 2.6.12 and Adv. Mater. **7,** 857 (1995).
[2] W. Bouwman and K. Kjær, Ann. Rep. Solid State Physics Dept., Risø, 1994, 2.6.1.

Annual Progress Report of the Department of Solid State Physics for 1996. Risø National Laboratory, Roskilde, Denmark (1997). Risø-R-993(EN). ISBN 87-550-2233-2. ISSN 0106-2840. ISSN 0907-0249.