22: X-ray scattering from films and superlattices

N. Boudet,

Institut Néel, CNRS and UGA

The study of thin films and superlattices has received an increased interest over the past years as a result of the wide range of interesting physical phenomena and properties observed in such systems. The nanometric scale and the periodic stacking of layers often lead to unique magnetic, transport and mechanical properties. Many applications for superlattices are being examined, e.g. mirrors for soft X-rays and neutrons, high critical current superconductors, magnetoresistive heads, ferroelectric memories or magneto-optical recording materials.

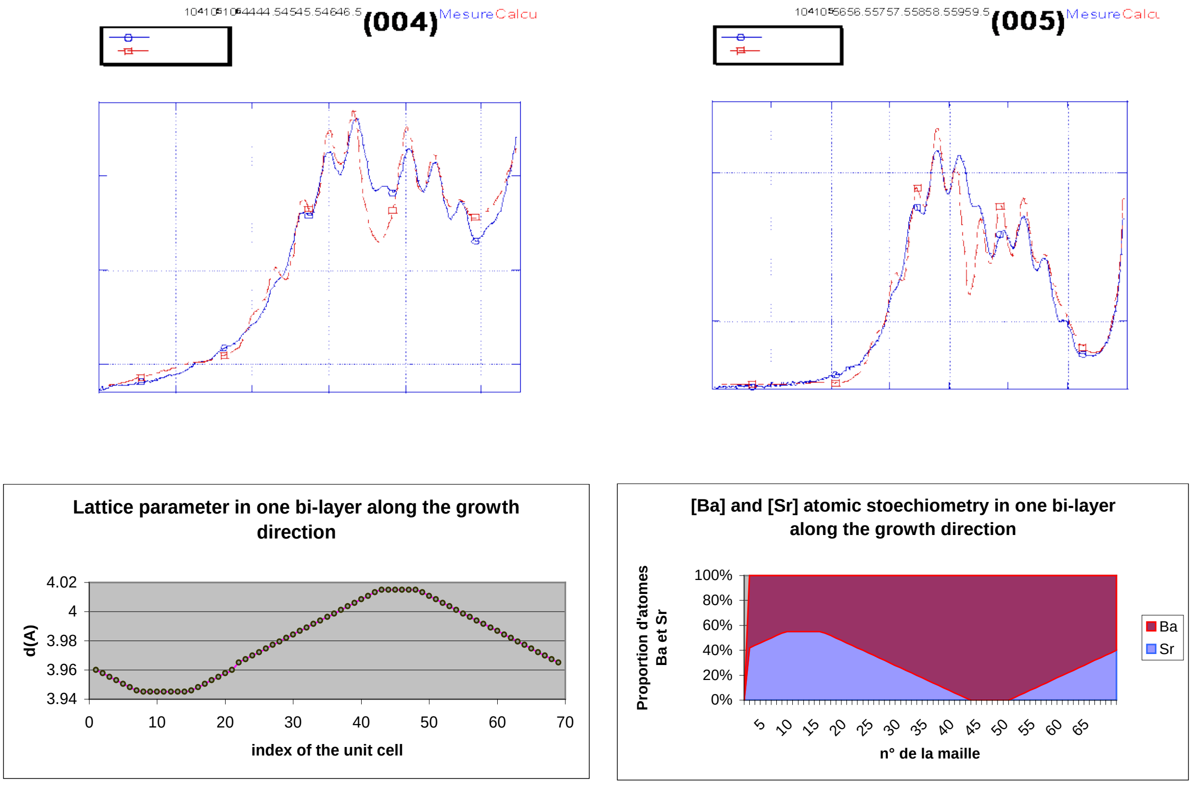

Figure 1. (00L) diffraction diagrams measured (continuous line) and calculated (dashed line) for a superlattice consisting of 15 bi-layers of (84 Å STO/ 193 Å BTO) (☐= 0,77485 Å), for L = 4 and 5. The bottom curves show the calculated average variation of the lattice parameter d(001) across a single bi-layer (left), and the calculated variation of the atomic proportions of Ba and Sr (with the constraint [Ba] + [Sr] = 1) along <001> in a single bi-layer (right).

Our understanding of such physical properties depends on the characterisation of the material. Many of the physical properties are function of the interfacial state and of the structural characteristics of the multilayered film such as interdiffusion, crystallinity, strain and roughness. X-ray diffraction is a well-suited technique for studying the structure of films and superlattices.

In these practicals, the sample is $(BaTiO_3/SrTiO_3)_{15}$ epitaxially grown by chemical vapour deposition of metallo-organic precursors (MOCVD) on a <001> oriented $SrTiO_3$ substrate. The sample will be mounted on a 7-circles high-resolution goniometer, at the D2AM/BM2 French CRG beamline at the ESRF. Reflection diffraction data (Fig. 1) along the growth direction (perpendicularly to the sample surface) and reciprocal space diffraction mapping (Fig. 2) will be carried out. Attention will be focused on the experimental principles of the data acquisition and the net advantage of using a synchrotron beam will be discussed. These measurements will then be related with the in-plane and out-of-plane microstructure of the material.

In a second part, the diffraction data will be processed, using a general kinematical diffraction model initially postulated by E.E. Fullerton and I.K. Schuller (Phys. Rev. B (1992) 9292). The model uses a variety of lattice parameter and concentration profiles, describing the strain and atomic diffusion from the interface to the core of each individual sub-layer. The model also includes statistical, continuous and discrete fluctuations around the average structure. This set of morphological parameters, describing the superlattice, is used for fitting the observed diffraction profiles in position, intensity and shape (Fig. 1).

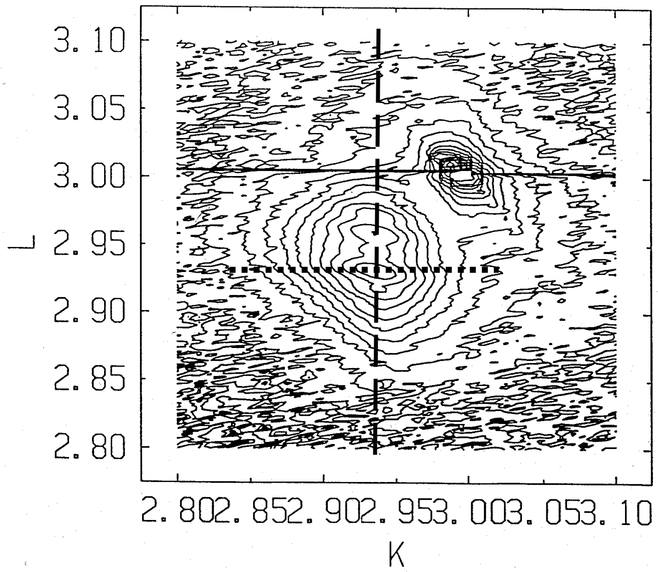

Figure 2. A superlattice composed of 15 bilayers of (84 Å STO / 193 Å BTO): *kl* reciprocal mapping around the diffraction node (*033)* showing the diffraction signal from both the superlattice and the substrate.

References

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