LONG-RANGE SCANS AND MANY-BEAM EFFECTS FOR HIGH-RESOLUTION X-RAY DIFFRACTION FROM MULTILAYERED STRUCTURES

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Thin crystalline films and multilayers are recently of wide use in modern nanoscale manufacturing in semiconductor, coating, optical and infrared industry. The broad use of these structures requires the adequate methods for characterization and quality control as well as for development of new electronic and optical devices with predictable properties.

A high dynamical range of X-ray measurements in modern instruments and synchrotron sources makes it possible to measure the diffraction peaks with a high accuracy and detailed fine structure, containing plenty of information. A special attention is paid to long angular range scans (LRS) containing multiple Bragg reflections, which deliver the comprehensive and consistent information on the investigated samples in a wide range of the sample crystallographic parameters. However, the complex scattering of X-rays within the sample in high-resolution LRS demands a precise theoretical interpretation of the measured data.

In present work, the multi-beam dynamical diffraction theory is proposed, which takes into account all the required corrections to provide a high accuracy of calculated diffraction spectra. The precision of the method is proved by comparison with experimental high-resolution X-ray diffraction scans from 22 nm $YBa_2Cu_3O_7$ layer on $SrTiO_3$ substrate, containing 16 Bragg reflections.