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Use of x-ray reciprocal lattice mapping for the characterization of single crystals and heterostructures

Reciprocal space mapping is a high-resolution X-ray diffraction method to measure a reciprocal space map (RSM). These maps around reciprocal lattice spots can reveal additional information beyond that provided by single line scans such as high-resolution rocking curves. RSMs are typically used to aid the interpretation of peak displacement, peak broadening or peak overlap. Several examples of RSMs for the characterization of single crystals and heterostructures will be given.

The relaxation of lattice strain in epitaxial buffer layers and virtual substrates is often accompanied by layer tilting, resulting in peak displacement. Bragg peaks of asymmetric reflections are also displaced in rocking curves as a result of epitaxial strain. Mismatch and threading dislocations in semiconductor epitaxial layers can give rise to peak broadening and peak overlap in traditional high-resolution rocking curve measurements. Measuring a reciprocal space map (RSM) is a way of separating these effects so that Bragg peak positions can be precisely measured. This is important for the determination of strain, lattice relaxation, composition and layer thickness in compound semiconductors, such as GaN-based devices for HEMTs and LEDs.

Reciprocal space mapping is particularly powerful for the general investigation of layer quality in thin layered structures. When there are defects in an epitaxial layer, it is broken into mosaic blocks which are perfect regions of crystal that are tilted or rotated with respect to each other. Similarly, crystal grains in polycrystalline deposited layers may share a common orientation. Reciprocal space mapping can be used to measure the size and relative tilts of mosaic blocks and to investigate texture in deposited films.

Epitaxial layers grown on substrates with a large lattice mismatch, such as GaN on sapphire, SiC on silicon, Ga_2O_3 on sapphire are characterized by a large defect density, generating a mosaic spread of the diffraction peak, and a broadening of the peak along the scattering vector. Usually in the papers the material quality is simply identified with the full width al half peak, but this parameter is affected by the instrumental resolution and it difficult to correlate it to the crystallographic quality of the material. The use of RSM permits to exactly distinguish between mosaic spread and crystallite dimensions in highly mismatched heterostructures. Reciprocal space maps can also clearly distinguish peak broadening arising from mosaicity from peak broadening due to other effects such as substrate curvature.