X-RAY DIFFRACTION PEAK PROFILES FROM RELAXED EPITAXIAL FILMS

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Epitaxial films relax because of the lattice parameter mismatch between the film and the substrate. Misfit dislocations are formed at the interface, and threading dislocations go from the interface to the surface. The x-ray diffraction peak profiles are sensitive to the dislocation strain fields and contain information on the dislocation densities, Burgers vectors, and positional correlations of the dislocations. The aim of this talk is to discuss main features of the diffraction patterns due to dislocations in epitaxial films, and demonstrate possibilities of obtaining information on dislocation distributions from the x-ray diffraction experiments [1]-[5].

Dislocations develop positional correlations to reduce elastic energy of the relaxed epitaxial film. The minimum of elastic energy of misfit dislocations is reached for periodic dislocations. The edge (Lomer) dislocations glide along the interface and can approach this state, while the 60° dislocations that glide in the inclined planes have less possibility to order. The case of large dislocation densities, when the mean distance between misfit dislocations is much smaller than the film thickness, is most important experimentally and relatively easy for calculations. Positional correlations are described by a single parameter $g \leq$ which is the mean-squared fluctuation of the number of dislocations on a given interval [1, 5]. The case of low dislocation densities is more complex and involves the correlation function for dislocation positions [3].

The positional correlations of threading dislocations are directed to screen the long-range strain fields of the dislocations. The x-ray diffraction profiles from threading dislocations in GaN epitaxial films [3] are well described by the Krivoglaz-Wilkens correlation function $G(x) \propto \exp[-\rho x^2 \ln(R/x)]$, where ρ is the dislocation density and R is a screening distance. From the fits of the experimental profiles, this distance occurs comparable with the mean distance between dislocations, so that just neighbor dislocations screen each other.

If statistical properties of the dislocation distribution are known (or postulated), the x-ray scattered intensity can be calculated by the Monte Carlo method [3]-[5]. The Monte Carlo integration is performed within the kinematical diffraction theory without any further simplifications or approximations. Dislocation positions are generated on random with desired positional correlations. The average over an ensemble of dislocations is performed by the Monte Carlo method. The spatial integration over the film can be performed either by the Monte Carlo method [3, 5] or by usual quadrature formulas [4].

The misfit dislocations are generated in the Monte Carlo calculations as Markov chains. A choice of the probability distribution for distances between neighbour dislocations allows a continuous variation from completely uncorrelated dislocations to almost periodic ones. The satellite reflections appear for highly enough correlations [3].

For threading dislocations, the screening of the long-range strain is provided by dislocation pairs with opposite Burgers vectors of two dislocations in the pair. The mean distance between dislocations serves as a screening distance. It can be larger than the mean distance between dislocations, so that the pairs overlap, rather than make separated dislocation dipoles [4].

Thus, the x-ray diffraction profiles can be evaluated for a wide class of distributions of misfit and threading dislocations in epitaxial films. A combination of the approximate calculations and the direct Monte Carlo modeling provides a solid ground for the dislocation density determination and the detailed description of dislocation distributions in relaxed epitaxial films.

References

[1] V.M. Kaganer, R. Köhler, M. Schmidbauer, R. Opitz, and B. Jenichen, *Phys. Rev.* ***B*** **55** (1997) 1793.

[2] V.M. Kaganer, O. Brandt, A. Trampert, and K.H. Ploog, *Phys. Rev.* ***B*** **72** (2005) 045423.

[3] V.M. Kaganer and K.K. Sabelfeld, *Phys. Rev.* ***B*** **80** (2009) 184105.

[4] V.M. Kaganer and K.K. Sabelfeld, *Acta Cryst.* ***A*** **66** (2010) 703.

[5] V.M. Kaganer and K.K. Sabelfeld, *Phys. Status Solidi* ***A*** **208** (2011) 2563.