# DIFFUSE X-RAY SCATTERING FROM DISLOCATIONS IN RELAXED SEMICONDUCTOR EPITAXIAL LAYERS – A MONTE-CARLO SIMULATION

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The analysis of diffuse X-ray scattering from imperfect crystals is usually based on the assumption that the diffracted wave is averaged over the statistical ensemble of all defect configurations. In this case the calculation can be done manually be means of well-known Krivoglaz theory. But very often we deal with the objects, which do not obey the averaging principles and require a specific approach for their description. We analyzed the intensity distribution of the scattered radiation without performing an ensemble averaging for the determination of densities of threading and misfit dislocations in relaxed GaN epitaxial layers and laterally patterned systems. Instead, we applied a Monte-Carlo simulation generating random positions and types of threading and misfit dislocations and numerically calculate the non-averaged amplitude of the scattering wave. Results of numerical simulations were compared with experimental data; this comparison demonstrates that the Monte-Carlo method can be used for the calculation of diffuse scattering from any type of defects in an epitaxial layer.

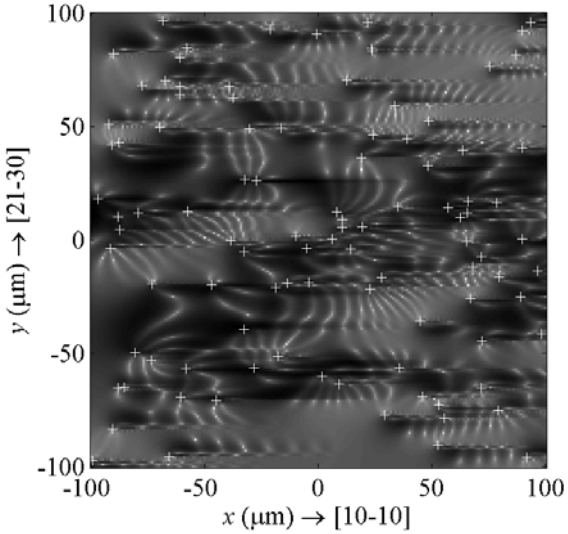


Fig. 1 Intensity distribution in the detector plane calculated for 100 randomly placed screw threading dislocations in a GaN(0001) layer, the crosses denote the dislocation positions, the sample is in the 0004 diffraction maximum.

[1] V. Holý, T. Baumbach, D. Lübbert, L. Helfen, M. Ellyan, P. Mikulík, S. Keller, S.P. DenBaars, and J. Speck, Phys. Rev. B **77**, 094102 (2008).

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