Integral equation based inverse diffraction problem solving for low-dimensional periodically-arranged nanocrystals

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Carrier confinement in low-dimensional periodically-arranged nanocrystals (LDPAN) leads to the dependence of the operating wavelength in LDPAN-based optoelectronic devices on the average size, shape, and material properties of heterostructures. Scatterometry as a non diffraction-limited optical method is applied to LDPAN (i.e. quantum dots, nanowhiskers, their combinations, etc) which are arranged on periodical masks. We propose numerical algorithms for the morphology determination of periodic relief nanostructures from light diffraction patterns measured in the UV–IR wavelength range. The solution of the direct 3D diffraction problem is reduced for some symmetrical LDPAN to the solution of boundary integral equations [1] for the 2D or even 1D Helmholtz equation. The ratio wavelength-to-period is small for typical inverse scattering problems and so the modified boundary integral equation method [2] has to be applied to obtain accurate results at a fast convergence rate for the direct problem [3]. The inverse problem is formulated as a non-linear operator equation in the Euclidean space with an assumed set of unknown structural parameters of nanocrystals (height, width, slope angles, and refractive indices) and a given set of determined efficiency and phase shift values. The operator maps the sought structural parameters to the amplitudes of diffraction orders. The present approach employs the gradient Levenberg-Marquardt method to solve the operator equation. This type of iterations is close to the Gauss-Newton method, but more efficient and stable for poor or improper input data [4] due to an additional regularization parameter. The inverse problem, mathematically, severely is ill-posed [5] and regularization techniques have to be used to improve the solution. Unfortunately, such a regularization is not enough even for simplest geometry considerations and serious restrictions to the number and values of reconstructed parameters must be applied. Here we consider problems with a few polygonal-type boundary profiles having several edge points only. The method can be applied to LDPAN grown in different material systems (group III-V, IV, II-VI, their combinations, etc) by various techniques (MBE, MOCVD, MOVPE, etc).

References

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