Optical characterisation of nanostructures using a discretised forward model

Optical diffraction microscopy (ODM) is a non-destructive and relatively inexpensive means of characterisation of nanostructures. It is an essential tool in the design, production and quality control of functional nanomaterials. In ODM, the target is reconstructed from the measured optical power in the reflected far field. This inverse scattering problem is typically highly ill-posed due to the incompleteness of the data and the low signal-to-noise ratio. In a realistic setting, the formulation of the forward scattering model is usually complicated by the presence of supporting structures (e.g., a substrate or a grid supporting a nanoparticle), since the electromagnetic interaction between the nanostructure and the supporting structure must be taken into account. Also, the roughness and the contamination of the supporting structure can increase the dimensionality and the ill-posedness of the inverse problem. Finally, the size of the measured nanostructure is typically comparable to the wavelength of the illuminating light, so the scattering needs to be described using the full Maxwellian electromagnetic model, rather than (numerically inexpensive) asymptotic formulations.

We here describe an efficient, accurate and robust forward scattering model [1,2] based on discrete sources and tailor-made for the reconstruction of 2D nanoparticles on substrates from ODM data. We adopt an analysis-based modelling paradigm, and attempt to incorporate as much available a priori information as possible directly in the forward model. We replace the classical radiation integrals by finite linear combinations of stratified Green's functions for the Helmholtz operator in the plane, and thus achieve a sparse formulation and an implicit description of the particle-substrate interaction. The forward model can be extended to include the roughness and contamination of the substrate without sacrificing the speed of computation [3]. We validate the model and show its feasibility in a decomposition-type inverse scheme with synthetic measurement data ([1], figure 1), as well as in the inversion of experimental scatterometric data ([4], figure 2). Finally, we use a related forward model in the inversion of synthetic measurement data to estimate aperiodic defects in a nanograting ([5], figure 3).

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This book studies methods to concretely address inverse problems. An inverse problem arises when the causes that produced a given effect must be determined or when one seeks to indirectly estimate the parameters of a physical system. The author uses practical examples to illustrate inverse problems in physical sciences. A numerical method based on a variational procedure, which allows the one-dimensional Schrödinger equation to be solved for an arbitrary potential energy function user-defined at selected mesh points, is used to construct an empirical one-dimensional vibrational potential for the double-well umbrella inversion problem in NH₃ and its isotopically substituted molecules. A numerical solution to the boundary inverse problem is determined by special decomposition which transforms the problem into two standard problems. We present the results of numerical experiments, including those with random errors in the input data, which confirm the capabilities of the proposed computational algorithms for solving this boundary inverse problem.

UDC 517.63. NUMERICAL METHOD FOR SOLVING BOUNDARY INVERSE PROBLEM FOR ONE-DIMENSIONAL PARABOLIC EQUATION V. I. Vasil'ev and Ling-De Su. Abstract. We consider a numerical method for solving boundary inverse problem using the implicit difference scheme for approximation by time and finite difference method for the boundary inverse problem.