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On a Fast Integral Equation Method for Diffraction Gratings

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Abstract. The integral equation method for the simulation of the diffraction by optical gratings is an efficient numerical tool if profile gratings determined by simple cross-section curves are considered. This method in its recent version is capable to tackle profile curves with corners, gratings with thin coated layers, and diffraction scenarios with unfavorably large ratio period over wavelength. We discuss special implementational issues including the efficient evaluation of the quasi-periodic Green kernels, the quadrature algorithm, and the iterative solution of the arising systems of linear equations. Finally, as an example we present the simulation of echelle gratings which demonstrates the efficency of our approach.

Key words: Diffraction gratings; integral equation method; preconditioning.

1 Introduction

For the numerical simulation of diffraction by optical gratings, several methods have been proposed, among them differential and integral methods, methods based on Rayleigh or eigenmode expansions, finite element or finite difference methods and methods of analytical continuation (cf., e.g., the Rigorous Coupled Wave Analysis [19], the C-Method [6], and the Finite Element Methods [2,3,8,27]). However, if the cross section of the grating geometry can be described by a small number of interface curves, then the approximation of the scattered electromagnetic field by an integral equation method is recommended. Integral equation methods are robust, reliable, and efficient. Such methods for calculating field components and efficiencies have been developed by e.g. Maystre, Pomp, Chen, Friedman,

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Prather et.al., Popov et.al., Yeung, Barouch, Goray, Sadov, and Kleemann (cf. [5, 12, 13, 18, 20, 22, 23, 29]).

Integral equation methods are well suited for the simulation of profile gratings with profile curves of arbitrary shape (cf. [13]). The grating materials can be dielectric or conducting, and profile gratings with coated layers can be treated as well (cf. [12, 20, 22] and the treatment of large numbers of layers in [11]). If the integrals occurring in the method are approximated by properly chosen quadrature rules, then coated layers with extremely small thickness are admissible. Even corners in the profile curve do not cause serious problems as long as the singular behavior of the electromagnetic field at the corner points is taken into account by the right discretization of the integral equations. More challenging is the treatment of gratings with large ratios period (grating constant) over wavelength. Such examples usually require numerical algorithms with large numbers of degrees of freedom, i.e., long computing times and huge storage capacities. Note, however, that surprisingly good results have been reported for the unconventional Modified Integral Method by Goray [10].

Integral equation methods can be considered as a special case of the so-called boundary element methods applied to boundary value problems for the elliptic Helmholtz equation. Consequently, the standard boundary element techniques can be utilized for the grating problems as well. This includes the choice of the discretization scheme and the quadrature rules and the adaption to corners and thin layers. Unfortunately, high ratios period over wavelength result in large wavenumbers which makes the fast iterative solution of the arising linear systems of equations or the implementation of fast methods like fast multipole or wavelet algorithms difficult. Though to our knowledge no attempt has been made to apply the fast boundary element techniques, we believe that they will be useful to design faster integral equation methods for gratings. Finally, let us stress one particularity of the grating problems in comparison to other boundary elements. The kernel functions are quasi-periodic Green's functions represented as infinite sums or integrals. Therefore, the kernel evaluation consumes a lot of computing time, and a fast but accurate evaluation algorithm is often the essential point in an efficient realization of the integral equation method (cf. the contributions by Sadov [25] and Linton [15]).

The subject of the present paper is to describe the recent improvements in the implementation of the integral equation package IESMP of the Carl Zeiss AG in Germany. These improvements enables IESMP to treat gratings with large ratios period over wavelength illuminated under large angles of incidence. Efficiencies of the reflected light in high orders can be determined. In addition, edges (corners of the profile curve in the cross section) and thin dielectric layers can be treated. For example, aluminum echelle gratings with aluminum oxide layers can be simulated. Following Pomp [20], we describe the integral equations for coated gratings and the numerical method in Section 2. In particular, section 2.4 contains some comments on the improved numerical scheme including a mesh grading at the corners. In Section 3.1 we present a new efficient way for the evaluation of the kernel functions inspired by Linton [15]. The new quadrature algorithm is given in Section 3.2, and the iterative solution of the discretized integral equations is discussed in