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Nuclear Instruments and Methods in Physics Research A 536 (2005) 211–221
NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A
www.elsevier.com/locate/nima

Numerical analysis of the efficiency of multilayer-coated gratings using integral method

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Received 29 June 2004; accepted 20 July 2004
Available online 17 August 2004

Abstract

An analysis is made of a rigorous and an approximate approach to the solution of the diffraction problem for a multilayer-coated X-ray grating by the integral equation formalism. Whereas a rigorous analysis involving the integral method requires a lot of computer resources, even for gratings with a small number of layers, the approximate approach based on a modification of the solution of the integral equation at the lower boundary with a finite conductivity is practically independent of the number of layers and is readily tractable with the use of a standard PC. The efficiencies of multilayer gratings measured at grazing angles with synchrotron soft X-ray radiation are compared with the values calculated using the integral approaches for ideal groove profiles.

PACS: 02.60.Nm; 07.05.Tp; 07.85.Fv; 42.40.Lx

Keywords: X-ray; Multilayer; Grating; Diffraction; Efficiency; Electromagnetism

1. Introduction

Multilayer-coated diffraction gratings offer the best promise for use in the short-wavelength range from hard X-ray to EUV, but modeling of their efficiency by rigorous methods meets with difficulties not encountered in calculation of bulk gratings [1]. The scalar theory of diffraction or application of the perfect conductivity approximation cannot predict exact results; especially, for grazing incidence angles, in the TM polarization, and in high orders. One may refer, for instance, to a rigorous calculation based on the differential method, but performed only for the ideal sawtooth profile with a small number of layers and only in the TE polarization [2]. The IESMP integral method is

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0168-9002/$ - see front matter
doi:10.1016/j.nima.2004.07.173

capable of handling bulk gratings with real groove profiles measured by scanning probe microscopy or any other modern tool [3]. The integral method is also applied successfully to studies of the efficiencies of so called lamellar multilayer amplitude gratings (LAMGs), which are the kind of the Bragg optics [4].

The present paper reports on an integral method applied to multilayer-coated gratings and referred to in the literature as "modified" [5,6]. It was employed to advantage to carry out the first calculation of the accurate efficiency of X-ray gratings with near-normal incidence, either coated by several layers or multilayered, with any groove profile, including a realistic (AFM-measured) groove shape [7,8], and with due account taken of random roughness [9–11]. The modified integral method permits easy modeling the efficiency of X-ray-range bulk real groove profile gratings operating at grazing incidence [12]. Application of the exact method requires, however, considerable computational resources, even in the case of gratings with a small number of layers. For instance, computation of one point for an X-ray grating with several tens of layers takes up many hours of work on a modern PC.

This stimulated the present author to develop in Section 2 along with the rigorous method an approximate approach for calculating the efficiency of grazing-incidence multilayer gratings, which is based on a modification of the solution to the integral equation at the lower finite-conductivity boundary and does not depend on the number of grating layers. A criterion of obtaining accurate data provided by the approximation to the integral method for multilayer X-ray grating efficiency calculations is proposed, and the conditions of its application are analyzed in Section 3. Next, in Section 4 the rigorously calculated and measured efficiencies of multilayer gratings with an ideal groove profile are compared with approximate data. Finally, the conclusion is given in Section 5.

2. A rigorous and an approximate approaches to calculate the efficiency of a multilayer grating

The coupled integral equations for a multilayer grating made up of K boundaries, starting with the top one (first), can be cast using the second Green's identity and boundary conditions, similar to the way this is done for a grating with one interface separating two media [10]:

$$\begin{aligned}
U_1(s_1)/2 = {} & U^i/2 + \int_{s_1} G_1^+(s_1, s_1')(c_j\, \mathrm{d}U_1(s_1')/\mathrm{d}n_1' \\
& - \mathrm{d}U^i(s_1')/\mathrm{d}n_1')\,\mathrm{d}s_1' \\
& + \int_{s_1} (\mathrm{d}G_1^+(s_1, s_1')/\mathrm{d}n_1')(U_1(s_1') \\
& - U^i(s_1'))\,\mathrm{d}s_1' \\
U_k(s_k)/2 = {} & \int_{s_k} c_j G_k^-(s_k, s_k')(\mathrm{d}U_k(s_k')/\mathrm{d}n_k')\,\mathrm{d}s_k' \\
& - \int_{s_k} (\mathrm{d}G_k^-(s_k, s_k')/\mathrm{d}n_k')U_k(s_k')\,\mathrm{d}s_k' \\
& + \int_{s_{k+1}} c_j G_{k+1}^+(s_k, s_{k+1}') \\
& \times (\mathrm{d}U_{k+1}(s_{k+1}')/\mathrm{d}n_{k+1}')\,\mathrm{d}s_{k+1}' \\
& + \int_{s_{k+1}} (\mathrm{d}G_{k+1}^+(s_k, s_{k+1}')/\mathrm{d}n_{k+1}') \\
& \times U_{k+1}(s_{k+1}')\,\mathrm{d}s_{k+1}' \\
U_{k+1}(s_{k+1})/2 = {} & \int_{s_{k+1}} c_j G_{k+1}^+(s_{k+1}, s_{k+1}') \\
& \times (\mathrm{d}U_{k+1}(s_{k+1}')/\mathrm{d}n_{k+1}')\,\mathrm{d}s_{k+1}' \\
& + \int_{s_{k+1}} (\mathrm{d}G_{k+1}^+(s_{k+1}, s_{k+1}')/\mathrm{d}n_{k+1}') \\
& \times U_{k+1}(s_{k+1}')\,\mathrm{d}s_{k+1}' - \int_{s_k} c_j G_k^-(s_{k+1}, s_k') \\
& \times (\mathrm{d}U_k(s_k')/\mathrm{d}n_k')\,\mathrm{d}s_k' \\
& - \int_{s_k} (\mathrm{d}G_k^-(s_{k+1}, s_k')/\mathrm{d}n_k')U_k(s_k')\,\mathrm{d}s_k', \\
U_K(s_K)/2 = {} & -\int_{S_K} c_j G_K^-(s_K, s_K') \\
& \times (\mathrm{d}U_K(s_K')/\mathrm{d}n_K')\,\mathrm{d}s_K' \\
& - \int_{S_K} (\mathrm{d}G_K^-(s_K, s_K')/\mathrm{d}n_K')U_K(s_K')\,\mathrm{d}s_K' \\
& k = 1, K-1;\, j = k-1, K
\end{aligned} \tag{2.1}$$

where s_k is the curvilinear coordinate of the boundary S_k, U^i is the incident field, U_k is the z-component of the electric or magnetic field at the kth boundary, $G_k^{\pm}$ is Green's function for the region above (+) or below (−) the kth boundary, $\boldsymbol{n}$ is the vector of the surface normal (directed from "−" to "+"), $c_j = 1$ for the TE polarization and