A rigorous method for random roughness accounting in X-ray–VUV ranges

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Multiple and multi-wave diffraction, refraction, absorption, and resonances influence significantly X-ray scattering from nano-irregularities of rough films. These are purely dynamical effects requiring rigorous theory to correctly describe the power change in the specular order and to give the nonspecular distribution with possible resonance peaks. Despite the considerable progress attained in the last decade in developing a rigorous theory for random roughness accounting, the author is aware only of approximated and asymptotic approaches for X-ray and neutron scattering such as the Born approximation and the distorted-wave Born approximation (DWBA). Even a general second-order theory of scattering from 1-D rough multilayers has not yet been developed.

The rigorous boundary integral equation method employed in the analysis of diffraction grating efficiency was extended recently to the case of non-periodical and quasi-periodical structures having roughnesses of any kind [1]. The PCGrate®-SX v.6.2 software developed allows one to operate with exact models (e.g. based on Maxwell's equations, rigorous boundary conditions, and radiation conditions) to study X-ray specular and non-specular scattering from rough bulk and multilayer structures in real space. For accounting random roughness rigorously in PCGrate 6.2 is used the model in which the randomly rough surface is represented by a grating of large period with a few or a large number of random asperities. So the program deals with a structure that is a grating from a mathematical point of view but that can model a random rough surface if the groove spacing becomes large compared with the correlation length of the random asperities. Moreover, if the width of the asperities has the same order of magnitude as the wavelength of incident light, the number of diffraction order is large, and the continuous speckle of the randomly rough surface is simulated by the discrete speckle of the grating. In order to compute the scattering properties of a rough surface using a forward electromagnetic solver, an ensemble of surface realizations must be generated and some averaging is required. The well-known spectral method is used in PCGrate 6.2.to generate a profile with a Gaussian height distribution and a Gaussian correlation function.

The present report dwells on an application of a comprehensive numerical analysis of X-ray scattering from single-boundary finitely conducting rough surfaces having asperities of different heights and correlation lengths, with the use of a mid-end workstation in a reasonable computation time. The difference between the two approximate and the rigorous approach can be clearly seen in Fig. which plots the calculated specular TE reflectivity of a gold mirror with different rms roughness σ and lateral correlation length L vs. angle of incidence for Cu $K\alpha_1$ radiation. For the Debye-Waller (DW) model $L = \infty$, for the Névot-Croce (NC) model $L = 0$, and for the rigorous model chosen $L = 5$ nm and $L = 500$ nm are close to ones used with the NC and DW models respectively.

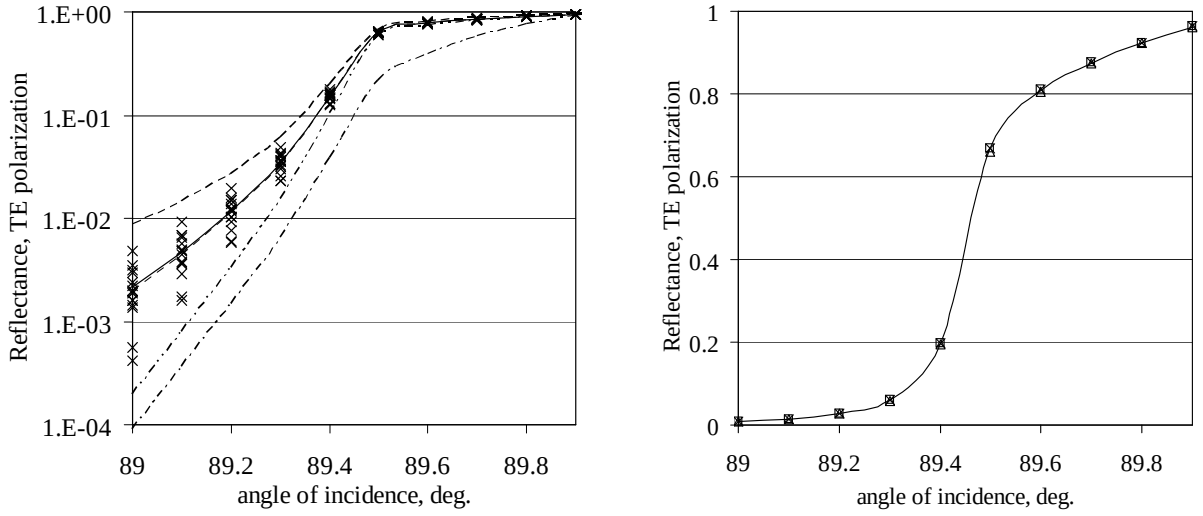

Fig. TE reflectance models of gold mirror calculated at λ = 0.1541 nm vs. angle of incidence for different σ and L. (left) σ = 0 and $L = \infty$ (long-dashed line – perfect surface); σ =1.5 nm and $L = \infty$ (long-short-dashed line – DW model); σ = 1.5 nm and $L = 0$ (long-two-short-dashed line – NC model); σ = 1.5 nm and $L = 5$ nm (markers × – rigorous model for different samples); σ = 1.5 nm and $L = 5$ nm (short-dashed line – rigorous average model for 10 samples); σ = 1.5 nm and $L = 5$ nm (solid line – rigorous average model for 15 samples). (right)) σ = 0 and $L = \infty$ (markers × – perfect surface); σ = 0.15 nm and $L = \infty$ (triangular markers – DW model); σ = 0.15 nm and $L = 0$ (square markers – NC model); σ = 0.15 nm and $L = 5$ nm (solid line – rigorous average model for 15 samples).

The difference between the rigorously and approximately calculated examples for σ = 1.5 nm is about an order of magnitude in the low reflectance range and about a few times in the intermediate range. In the high reflectance range for σ = 1.5 nm and especially for σ = 0.15 nm in the whole reflectance range, the difference between the rigorous and NC models is much smaller. The rigorously calculated specular reflectances lie between the estimates made with the NC model and those for a perfect (non-rough) mirror; this implies that the NC factor overestimates the influence of roughness, and that the rms roughness values σ obtained by fitting experimental data to the NC approximation are too small for grazing angles higher than the critical angle. This conclusion can be drawn also from the validity range derived for the NC factor and for the first- and second-order DWBA theory.

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[1] L. I. Goray, "Rigorous solution for electromagnetic scattering from multilayer structures having asperities of any kind in X-ray–EUV ranges," SPIE Proc. 6617, 2007, p. 661719.