Accurate computation of the X-ray diffraction efficiency of a multilayer coated grating based on a non-conformal deposition model

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In the 1-5 keV energy range where penetration depth can be significantly large, a multilayer stack deposited on a shallow modulated grating behaves as a double periodic medium and can provide enhanced Bragg reflectivity in proper tuning conditions[1,2]. For several years now, SOLEIL has undertaken to include multilayer coated grating in some of the beamline monochromators to extend the range of energies on soft X-ray or hard X-ray beamlines.
The latest realization was a Cr/B_4C multilayer grating for SOLEIL Sirius beamline. The 6.3 nm period multiyear stack was deposited at Laboratoire Charles Fabry on a 2400 l/mm grating with a 3.3 nm high lamellar profile ion-etched in Si by Horiba Company. The diffraction efficiency of this grating has been extensively measured with the goniometers available at SOLEIL, namely from 500 eV to 1500eV on the Metrology low-energy beamline branch and from 2000 eV to 4400 eV both on Metrology high energy branch and Sirius beamline itself with its crystal monochromator.
These measurements have shown a qualitative agreement with simulations produced with the CARPEM diffraction code[3] and a simple model assuming the conformal replication of a perfect rectangular profile throughout the layer stack and 3 discrete layers per period, the 3rd layer being introduced to account for the diffusion of B_4C in a an underlying Cr layer[4]. An arbitrary 0.8 reduction factor had to be applied to the calculated efficiencies to compensate the model imperfection but some features still could not be explained. The conformal model was also contradicted by AFM measurements of the grating surface which showed that the lamellar profile before coating was turned into an almost sinusoidal one after coating.
To overcome these issues a new grating model was developed and the CARPEM code was substantially modified to handle it. This new model is continuous and accounts for interfacial roughness and interdiffusion. It is also non-conformal. We consider that the local deposition rate is affected by surface tension and increased or reduced by a term proportional to the local curvature of the surface $\frac{\partial Z(x,t)}{\partial t} = v_0\left(1 + k\ \frac{\partial Z}{\partial x^2}\right)$. When the growth interface is under tension, k is positive and the high Fourier components of the surface modulation are damped proportionally to the square of their rank, turning the surface grating to sinusoidal. We show that this model explains all features of the measured data, the refraction shift of diffraction angles, the 55% maximum efficiency at 4100 eV, the reduced efficiency at low energies and even a glitch at 4400 eV which is not predicted by the conformal model. Moreover only the damping k parameter had to be fitted, the multilayer parameters, material densities, interfacial roughness and diffusion length being deduced from Cu K_α reflectivity measurements of a witness mirror coated with the same multilayer.

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[3] A. Mirone, et al., Appl. Optics **37**(25), 5816-5822 (1998)
[4] C. Burcklen et al., Journal of Applied Physics 119, 125307 (2016)