Characterizing profile tilt of nanoscale deep-etched gratings using Mueller matrix spectroscopic ellipsometry

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We are proposing to fabricate hundreds of high-efficiency critical-angle transmission (CAT) gratings to cover the large aperture of telescopes used in high spectral resolution x-ray astronomy[1]. The gratings are high-aspect-ratio (HAR), monolithic structures fabricated from silicon-on-insulator (SOI) wafers (Figure 1). We blaze into high diffraction orders by ensuring the grating bar sidewalls are aligned with incident x-rays at an angle below the critical angle for total external reflection ($\theta_c \sim 2^\circ$). This not only increases diffraction efficiency by maximizing external reflection, but also yields higher resolving power by increasing the angular separation between neighboring wavelengths[2]. To optimize blazing into high diffraction orders we require a nearly constant ($\Delta\theta \leq 0.2^\circ$) incident x-ray angle across a grating, but have found that for some tools the deep reactive-ion etching (DRIE) process necessary for producing HARs yields significant bar tilts (~0.07°/mm, up to 3.5° across 50 mm) away from the wafer surface normal. We previously developed a method[3] to measure these tilts with small-angle x-ray scattering (SAXS), but the process is destructive and requires several days per wafer. We present a fast, nondestructive optical technique to characterize tilt based on Mueller matrix spectroscopic ellipsometry (MMSE). We first capture experimental MMSE spectra from the sample grating we wish to characterize. We then build a model of our grating in a commercially available RCWA-based EM solver (Figure 2), computing associated model Mueller matrix spectra (Figure 3). The model has several free parameters, one of which is the bar tilt. We expect our model parameters to approach those of our sample as their respective spectra converge. We therefore use nonlinear regression (Levenberg-Marquardt) on the free parameters to minimize the mean squared error between the experimental and model spectra. Once the minimization terminates, we extract the model tilt parameter and use it as our measurement of the sample tilt. We validate our method by measuring tilt on a physical wafer with SAXS (Figure 4). The speed of this technique in principle allows in-line tracking and tuning of etch processes.

[1]Heilmann, R. K., Bruccoleri, A. R., Kolodziejczak, J., Gaskin, J. A., O'Dell, S. L., Bhatia, R., & Schattenburg, M. L. (2016, July). Critical-angle x-ray transmission grating spectrometer with extended bandpass and resolving power> 10,000. In Space Telescopes and Instrumentation 2016: Ultraviolet to Gamma Ray (Vol. 9905, pp. 553-564). SPIE.
[2]Heilmann, R. K., *et al*. (2018, July). Blazed transmission grating technology development for the Arcus x-ray spectrometer Explorer. In Space Telescopes and Instrumentation 2018: Ultraviolet to Gamma Ray (Vol. 10699, pp. 1518-1529). SPIE.
[3] Song, J., Heilmann, R. K., Bruccoleri, A. R., & Schattenburg, M. L. (2019). Characterizing profile tilt of nanoscale deep-etched gratings via x-ray diffraction. Journal of Vacuum Science & Technology B, 37(6).

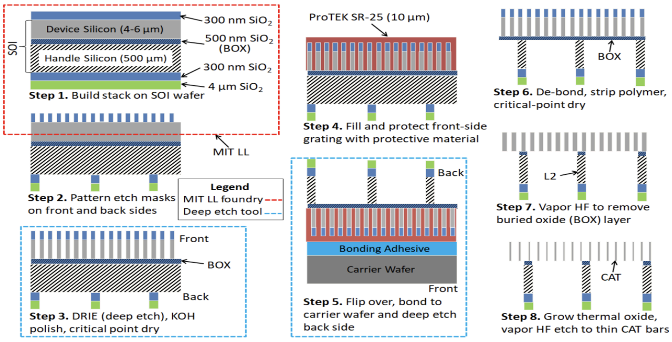

Figure 1: Simplified illustration of the CAT grating fabrication process.

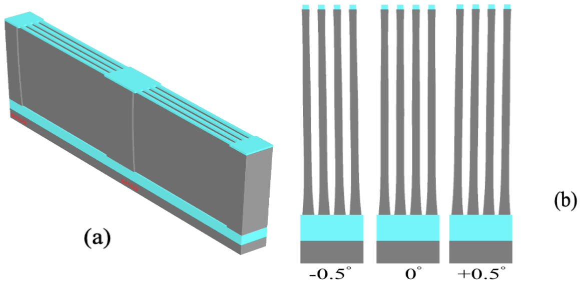

Figure 2: (a) 3D model of CAT grating structure. (b) Cross sectional view of 4 µm-deep, 100 nm-line/space CAT grating structure at various tilt angles.

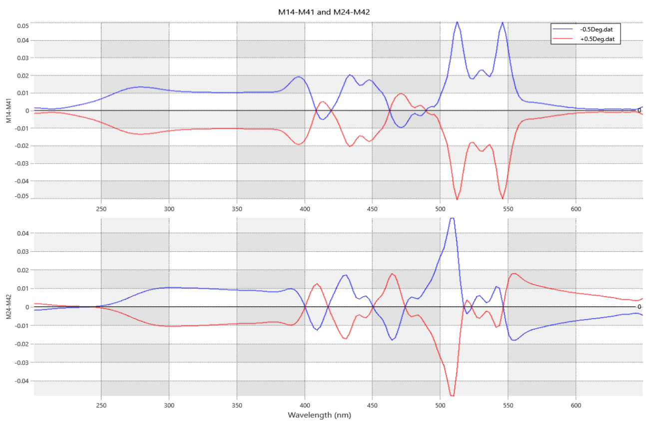

Figure 3: Simulated, model Mueller matrix spectra plotting two matrix elements against wavelength (nm) for symmetric tilt angle perturbations (+0.5°, -0.5°). The sensitivity of the Mueller matrix spectra to tilt is apparent.

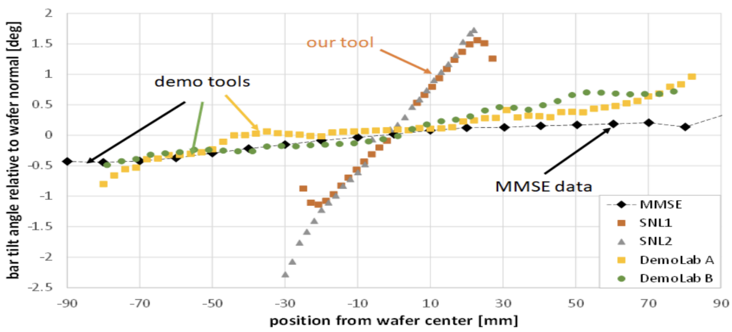

Figure 4: Measured bar tilt angle vs. position across different wafers using SAXS and MMSE methods, on gratings etched with a variety of DRIE tools.