Simulation of "Spectral Ghosts" Generated by Imperfectly Fabricated Diffraction Gratings

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High resolution (R>10,000) spectra are of critical importance to a number of research fields including astronomy and synchrotron beamline science. To create these spectra, modern spectrometers often require precisely fabricated, custom, large-area (>50 cm^2) diffraction gratings with high groove densities (1000s gr/mm), critical dimensions <1 micron, and low line edge roughness. Direct-write techniques, such as electron beam lithography (EBL), are thus a preferred fabrication method due to the technique's precision and adaptability[1,2]. Motivated by these requirements and an ultraviolet astronomy use-case, we have fabricated gratings via EBL and seek to fully characterize their performance with special attention to spectral defects caused by feature placement errors in the patterning process.

Feature misplacement is of particular importance since these errors, often caused by field-to-field stitching or drift, can cause groove discontinuities resulting in phenomena known as Rowland and Lyman Ghosting. "Ghost" orders refer to a multiplicity of a single spectral order which manifests due to incident light diffracting at more than one effective period (Fig. 1). This degrades the overall quality of the spectrum, regardless of the grating's resolution and efficiency, due to a degeneracy in the location of wavelength-specific peaks at the observation plane. To quantify the appearance of ghost orders, we use interferometric measurements of the grating's period error[3] to simulate the intensity distribution generated by the imperfect grating. This technique enables an iterative process for exploring critical tolerances of feature placement accuracy when designing and patterning gratings over large areas. We report on progress using interferometric metrology and a Fourier optics mathematical approach to simulate and quantify the ghosting effects of discontinuities on real gratings fabricated via EBL.

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[1] Zeitner, U.D., Oliva, M., Fuchs, F. *et al.* High performance diffraction gratings made by e-beam lithography. *Appl. Phys. A* **109**, 789–796 (2012). https://doi.org/10.1007/s00339-012-7346-z

[2] Fabien Grisé, Nicholas Kruczek, Brian Fleming, Randall McEntaffer, Drew M. Miles, Chad Eichfeld, Michael Labella, and Kevin France "Fabrication of custom astronomical gratings for the extreme and far ultraviolet bandpasses", Proc. SPIE 11821, UV, X-Ray, and Gamma-Ray Space Instrumentation for Astronomy XXII, 1182112 (24 August 2021); https://doi.org/10.1117/12.2594796

[3] DeRoo, C. T. et al. 2020, "Limiting spectral resolution of a reflection grating made via electron-beam lithography," The Astrophysical Journal, 905(1), 2020 https://doi.org/10.3847/1538-4357/abbe15

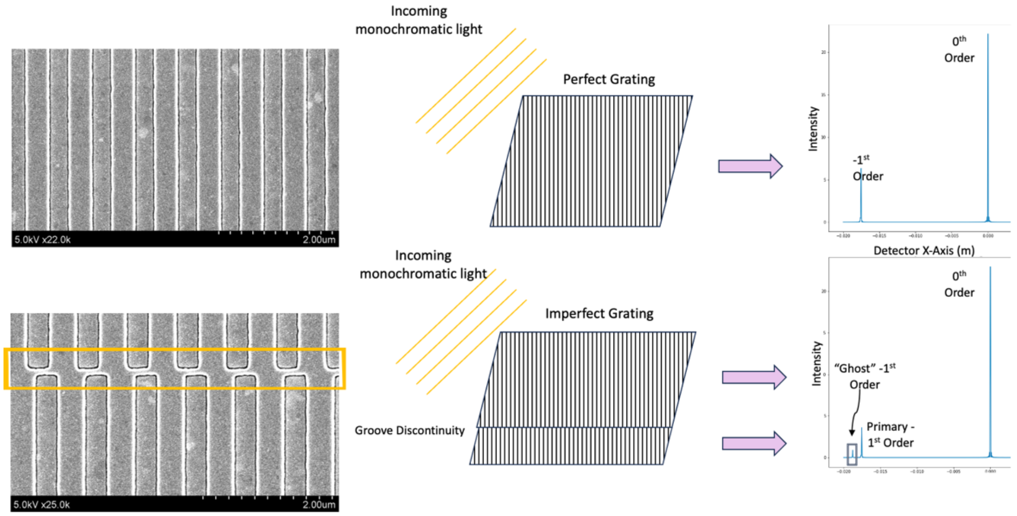

Figure 1: (Left) Scanning electron micrographs of a grating with and without groove discontinuity. (Center) Cartoon of light incident on each type of grating. (Right) Simulated intensity distribution showing a perfectly ideal case with a single -1st order (top) and the appearance of a ghost order (bottom).