Multilayer Optics for Mo Radiation based X-ray Crystallography

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The fabrication of multilayer optics for Mo Kα, the wavelength of choice for small molecule crystallography, is difficult because for this wavelength the maximum angles of incidence at which a multilayer reflects and the Bragg peak widths are small. Consequently, only a small solid angle and a small fraction of the X-ray source can be captured. The resulting intensity gain compared to a graphite monochromator is often disappointing. However, today's deposition techniques allow for the fabrication of high quality multilayers with a small d-spacing that reflect at large angles of incidence. The resulting capturing angles are large enough to produce intense beams.

In this work we designed, fabricated and evaluated a focusing multilayer optic for Mo Kα X-rays. The optic was comprised of two elliptically bent focusing multilayers, which were arranged in the Montel scheme. The paper shows the design and performance of the optic. For an FR591 rotating anode X-ray generator, a comparison of the multilayer optic with a graphite monochromator showed a 5x intensity enhancement. Especially small and weakly diffracting crystals benefit from the large intensity produced by the optic, as illustrated by diffraction analyses. An application case study using a small crystal showed significantly improved resolution, with $\langle I/\sigma \rangle$ values larger than 10 for resolution shells down to 0.77 Å where $\langle I/\sigma \rangle$ was only 1.5 for the graphite monochromator. The R indices improved by a factor 3 when data down to 0.77 Å were used for the evaluation.

Keywords: multilayer x-ray optics, single crystal x-ray crystallography, small molecules