Internet-Based X-ray Server

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X-ray Server is a public project for online analysis of X-ray diffraction and scattering data that recently passed the milestone of 100,000 calculations. The aim of this project is to explore novel opportunities given by Internet for sharing research results with wide scientific community, establishing collaborations, and refining scientific software. The Server provides Web-based access to a number of data analysis programs based on author's publications in the fields of X-ray optics and X-ray material science. The software operates directly on the Server available for use without downloading. This has proven to be the most efficient technology for having feedback from users and refining and extending the software. The advantages on users' side are also essential as confirmed by the Server success. Currently Server programs provide: (1) Interpolating X-ray dispersion corrections from discrete sets with an original algorithm; (2) Calculating X-ray rocking curves from strained crystals and multilayers for any Bragg-case diffraction including grazing incidence and/or exit and with scans around arbitrary axes; (3) Calculating X-ray specular reflection from multilayers with interface roughness using new recursive algorithm converging faster than the Parrat recursions; (4) Calculating X-ray resonant specular reflection from magnetic multilayers with magnetic interface roughness; (5) Calculating X-ray diffuse scattering from correlated interface roughness in multilayers; (6) Calculating multiple Bragg diffraction of X-rays with the help of new algorithm applicable to grazing incidence and/or exit. The report overviews the Server structure and the physical models beneath the server programs and demonstrates some applications.

Keywords: simulation x-ray diffraction, web internet techniques, x-ray diffraction theory