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Accurate Ray Tracing of Bent Crystals in Bragg and Laue Geometries in Real Time with xrt and OpenCL

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One of the major advantages of the *xrt* ray tracing and wave propagation package is its precise quantitative representation of the material properties of an optical element. *xrt* supports various kinds of X-ray optics including reflective (mirrors, capillaries), refractive (lenses), and dispersive (crystals, multilayers, zone plates and gratings). Complex amplitudes of reflectivity or transmittivity are calculated on the fly for a given set of direction, energy, and polarization, characteristic to an individual ray, thus eliminating the need for pre-calculated reflectivity maps and subsequent interpolation.

When it comes to the accurate calculation of the reflectivity of a bent crystal, either in Bragg or Laue geometry, there is no simple analytical solution. In the most general case, one would need to solve a system of ODEs called the Takagi-Taupin equations (TTE) numerically. A number of approximations have been developed over the years, including the Multi-Lamellar (for both Bragg and Laue cases) and the Penning-Polder (Laue only) models. Although not as precise as the TTE, they still pose a certain computational challenge.

In our work, we aimed to maintain the precision of the TTE method while increasing the performance to a level sufficient for real-time ray-tracing. We applied the adaptive Dormand-Prince method to calculate the amplitudes of forward-propagating and reflected waves inside a bent crystal and used the OpenCL framework to accelerate calculations. We rely on the pyTTE package to calculate a) elastic constants, required for integration, for a number of predefined crystals, such as Silicon, Germanium, Diamond, Alpha-Quartz, and some others, and b) the local orientation of the diffracting planes inside a crystal. The latter enables us to simulate phenomena such as monochromatic and polychromatic focusing, as well as sagittal focusing in asymmetrically cut Laue crystals. Performance-wise, we can process tens to hundreds of thousands of samples (rays) per second on a consumer-grade GPU.

The correctness of the calculations has been verified by a series of measurements performed at the BXDS beamline, Canadian Light Source, for a variety of asymmetrically cut Silicon crystals in Laue geometry.

Fig.1 Volumetric diffraction in asymmetrically cut Si[111] crystal with anticlastic bend, Laue geometry

I plan to submit also conference proceedings

Yes

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