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Modeling X-ray diffractomerers using ray tracing and parallel coprocessors

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In X-ray powder diffraction, the use of the Rietveld technique to refine crystalline structures requires modeling the diffractometer. Some of the codes using this technique incorporate simple models for it. These codes do not affect the refined parameters only when the X-ray source is a synchrotron with enough X-ray optic to reduce the associated aberrations. When the diffractometer belongs to a standard laboratory, however, the optic associated to it gives rise to large aberrations; for example, asymmetric and shifted peaks that depend on the diffraction angle. When the above codes are used to refine crystalline structures, the refined parameters are non-confident, because they are partially modeling these aberrations. If in the code, the effect of the optical components on the diffraction pattern is modeled correctly, the obtained refined parameters will be more confident. This kind of modeling has been done in the codes that use the fundamental parameters model for the diffractometer. There are two ways to perform this modeling: in one of them the codes use an analytical model for each one of the optical components of the diffractometer; other codes use the ray tracing technique to model the path of the x-rays along the optic. This last technique requires a powerful computer facility. In this work, we present the developing of an open-source code to model the diffractometer by using the ray tracing technique. To reduce the calculation time, the code was written in OpenCL for a computer with a Fermi K20 coprocessor, and for a computer with a Xeon-Phi coprocessor, using the Qt platform for both systems. The device-function generated with this code can be used as input for any other code that models diffraction patterns, or refines crystalline structures. The code can also be used for teaching the effect of the different optical components on an X-ray powder diffraction pattern, including the effect of a wrong alignment of these components.

Keywords: ray tracing, X-ray diffractometer, Rietveld