An Advanced Computer App for Simulating White-Beam Diffraction Laue Patterns in Modern X-Ray Crystallography

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X-ray diffraction is the most common technique for determining atomic structures of crystals (e.g. semiconductors and proteins), and white-beam diffraction is such a powerful method that]produces the Laue pattern (LP) by diffraction from different lattice planes simultaneously. However, interpretation of LPs is impossible by hand, which is an enduring challenge in history. This project is to create a fundamental computer program, called LauePt4, that simulates LPs of any crystals. It calculates the diffraction vector and reflection direction of each lattice plane and determines the diffraction spot on the recording detector. It has friendly graphic user interfaces that allows free crystal rotation while instantly simulating the LP overlapped on the recorded LP. A key obstacle in crystallography is the difficulty of recognizing a LP from a crystal with unknown orientation. LauePt4 features three novel strategies that solve this historic problem. First, LauePt4 allows the user to select a diffraction G vector and rotate the crystal around it by 360 degrees, which reduces the number of trial simulations for finding the match from millions to hundreds. The second and third strategies are automatic searching schemes that use selection of two or three spots. Then LauePt4 finds all the lattice plane pairs or triplets satisfying the interplanar angles and simulates the LPs to quickly find the match. LauePt4 can be used to rapidly identify crystals, their orientations, atomic structures, defects, and other information critical to materials science. LauePt4 has already been widely used by scientists at National Laboratories for studying SiC and GaN semiconductors that are critical to emissions-reducing renewable electric vehicles, 5G networks, and Air Force AESA radar technology.

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