New Modeling Tool Developed For Imaging Atomic Displacement in Crystals

Scientific Achievement

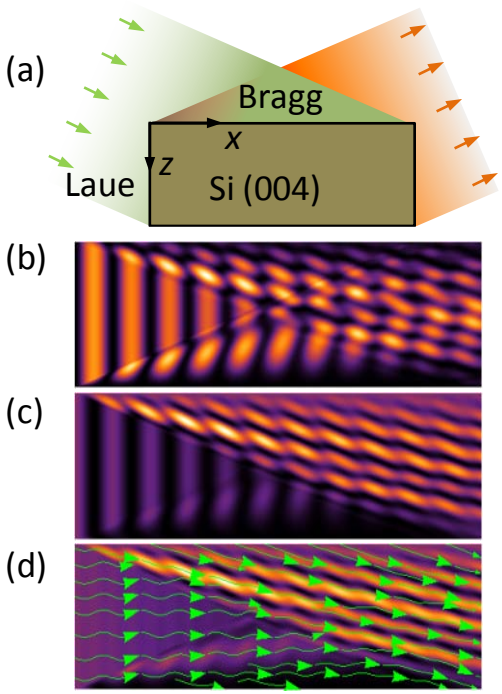
Scientists have developed a new method to model x-ray dynamical diffraction.

Significance and Impact

Dynamical diffraction theory is fundamental in x-ray scattering science. This new theoretical model opens up opportunities to explore new ways of measuring strain in crystals. It also sheds light on fundamental diffraction problems that have not been fully understood before.

Research Details

- Strain can affect optical, mechanical and electrical properties of crystalline materials. Correct strain imaging is vital to understanding the underlying physics.
- This theoretical development will enable scientists to correctly image structural changes in single microcrystals at spatial resolutions ranging from 10 to 30 nanometers, with the long-range goal of 1 nanometer using the HXN beamline at the National Synchrotron Light Source II.



(a) Schematic of a silicon microcrystal illuminated by 12 keV x-rays. Dynamical diffraction in Bragg and Laue geometries are excited simultaneously.
(b)-(d) Simulated results are shown of the diffracted wave, the transmitted wave, and the energy flow (in the direction of the green arrows), respectively.

H Yan and L Li, *Physical Review B* 89, 014104 (2014)

Work was performed at Brookhaven National Laboratory