Abstract Submitted
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Quantifying defect levels in hexagonal boron nitride from simulated x-ray absorption spectroscopy[1] SEBASTIAAN HUBER, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, United States, ROBBERT VAN DE KRUIJS, FRED BIJKERK, Industrial Focus Group XUV Optics, MESA+ Research Institute for Nanotechnology, University of Twente, The Netherlands, ERIC GULLIKSON, Center for X-Ray Optics, Lawrence Berkeley National Laboratory, Berkeley, United States, DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, United States — X-ray Absorption Spectroscopy is a technique that is highly sensitive to the local structural and chemical environment of the probed species. This quality can be exploited to investigate the characteristics of localized structural imperfections such as point defects and grain boundaries. In this study the X-ray absorption spectra for various hexagonal (h-BN) and amorphous boron nitride (a-BN) samples have been recorded. Simulation of X-ray absorption spectra from first principles allows for characteristic features in the measured spectra to be attributed to local defects of the planar hexagonal structure of the material. Analysis of the relative intensities of these features can subsequently provide a quantitative analysis of the levels of various defects in the analyzed structure.

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