

MONASH CENTRE FOR ELECTRON MICROSCOPY

Atomic Column-by-Column Imaging of Atomic Vibrations Using Segmented and Pixelated Detectors

Date: Monday 10 February

Time: 4pm to 4:30pm

Venue: School of Physics and Astronomy,

Large Seminar Room, 10 College Wlk, Clayton-1-107

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Koudai Tabata is a PhD student at the University of Tokyo, working on the development of new STEM imaging techniques. His research interests currently encompass the development and application of atomic-scale thermal vibration imaging by STEM, as well as the integration of computational science.

Abstract

Aberration-corrected scanning transmission electron microscopy (STEM) is a powerful technique for directly visualizing atomic structures and local chemistry. Annular dark field (ADF) STEM, widely used for atomic-scale investigations, primarily detects thermal diffuse scattered electrons originating from atomic displacements, particularly those induced by atomic vibrations[1]. However, conventional annular detectors lack the spatial resolution to capture fine details of thermal diffuse scattering patterns, limiting their ability to resolve anisotropic atomic vibrations.

Recent advances in fast segmented and pixelated detectors have enabled detailed analysis of electron scattering distributions associated with atomic vibrations. In this study, we employed a segmented detector in STEM to identify anisotropic thermal diffuse scattering, revealing anisotropic atomic vibrations in the clathrate compound $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$ at atomic resolution[2]. Furthermore, atomic displacements of heavy elements in clathrate compounds were quantitatively characterized through simulations incorporating atomic displacement parameters that account for the anisotropic nature of atomic vibrations.

In contrast, pixelated detector, which capture more detailed distributions of thermal diffuse scattered electrons, are expected to be a powerful tool for probing atomic vibration-related physical properties, such as localized phonons. However, the large data volumes generated by pixelated detectors necessitate efficient methods for extracting atomic vibration parameters from experimental observations.

Automatic differentiation, a computational technique for efficiently and accurately computing derivatives of functions expressed in computer programs, has been widely adopted across various scientific fields. In this study, we developed a differentiable STEM image simulation package to facilitate parameter optimization and explored a framework for estimating atomic vibration parameters from data acquired with pixelated detectors.

References:

1. S. J. Pennycook et al., Ultramicroscopy 37 (1991), p. 14-38. [https://doi.org/10.1016/0304-3991\(91\)90004-P](https://doi.org/10.1016/0304-3991(91)90004-P)
2. K. Tabata et al., Small Sci 4 (2024), 2300254. <https://doi.org/10.1002/smssc.202300254>

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