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Characterizing crystalline defects in single Xe nanoparticles from angular correlations of single-shot diffracted X-rays

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Synopsis We performed a wide-angle X-ray scattering experiment of single Xe nanoparticles using an X-ray free electron laser. We developed a novel analysis method that focuses on the angular correlation between plural Bragg spots in single-shot diffraction patterns. The angular correlations of the Bragg spots encode rich structural information and offer an evidence of twinning and stacking faults in Xe nanoparticles.

Characterizing crystalline defects in nanoparticles is of crucial importance for their applications in science and technology, since the defects potentially alter their desired properties. Single-shot X-ray diffraction with X-ray free electron lasers (XFELs) is a promising method to investigate the structure of nanoparticles, in which diffraction patterns of single nanoparticles are obtained with exposures to single XFEL pulses.

In this study, we carried out a wide-angle X-ray scattering experiment on Xe nanoparticles at an XFEL facility SACLA [1] in Japan. Single Xe nanoparticles (average radius $r \sim 65$ nm) were irradiated by 11.2-keV XFEL pulses, and the diffracted X-rays were recorded on a shot-by-shot basis with a multiport CCD sensor detector. The diffraction patterns contain Bragg spots corresponding to $\text{fcc}\{111\}$, $\{200\}$, $\{220\}$ and $\text{hcp}\{101\}$

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reflections.

In order to extract further structural information from the single-shot diffraction patterns, we developed an analysis technique that focuses on angular correlations [2] between plural Bragg spots in single-shot diffraction patterns. The analysis has revealed clear angular correlations between the Bragg spots, which provide rich structural information on the nanoparticles. We carried out a simulation to quantitatively evaluate the angular correlations and obtained a solid evidence of twinning and stacking faults in the Xe nanoparticles.

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References

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