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A Niozu[1,2]*, Y Kumagai[3], T Nishiyama[1,2], H Fukuzawa[2,3], K Motomura[3], M Bucher[4], Y Ito[3], T Takanashi[3], K Asa[1,2], Y Sato[1,2], D You[3], Y Li[3], T Ono[3], E Kukk[5], C Miron[6,7], L Neagu[7,8], C Callegari[9], M Di Fraia[9], G Rossi[10], D E Galli[10], T Pincelli[10], A Colombo[10], T Kameshima[11], Y Joti[11], T Hatsui[2], S Owada[2], T Katayama[11], T Togashi[11], K Tono[11], M Yabashi[2], K Matsuda[1], C Bostedt[4,12,13] K Nagaya[1,2] and K Ueda[2,3]

[1]Division of Physics and Astronomy, Kyoto University, Kyoto 606-8501, Japan
[2]RIKEN SPring-8 Center, Sayo, Hyogo 679-5148, Japan
[3]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan
[4]Chemical Sciences and Engineering Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, USA
[5]Department of Physics and Astronomy, University of Turku 20014 Turku, Finland
[6]LIDYL, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette, France
[7]Extreme Light Infrastructure - Nuclear Physiscs (ELI-NP), "Horia Hulubei" National Institute for Physics and Nuclear Engineering, 30 Reactorului Street, RO-077125 Măgurele, Jud. Ilfov, Romania
[8]National Institute for Laser, Plasma and Radiation Physics, 409 Atomistilor PO Box MG-36, 077125 Magurele, Jud. Ilfov, Romania
[9]Elettra - Sinchrotrone Trieste, 34149 Basovizza, Trieste, Italy
[10]Department of Physics, Universitá degli Studi di Milano, Via Celoria 16 - 20133 Milano, Italy
[11]Japan Synchrotron Radiation Research Institute (JASRI), Sayo, Hyogo 679-5198, Japan
[12]Laboratory for Femtochemistry, Paul-Scherrer Institute, CH-5232 Villigen PSI, Switzerland
[13]Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

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 corresponing to fcc{111}, {200}, {220} and hcp{101} 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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*E-mail: niozu.akinobu.85s@st.kyoto-u.ac.jp