

PAPER • OPEN ACCESS

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

To cite this article: A Niozu *et al* 2020 *J. Phys.: Conf. Ser.* **1412** 202028

View the [article online](#) for updates and enhancements.

A promotional banner for the 240th ECS Meeting. The banner features a colorful striped border at the top. On the left, the ECS logo is displayed in a green circle. To its right, the text reads "240th ECS Meeting" in large blue font, followed by "Oct 10-14, 2021, Orlando, Florida" in a smaller blue font. Below this, it says "Register early and save up to 20% on registration costs" in bold black font, and "Early registration deadline Sep 13" in a smaller black font. At the bottom left, there is a red "REGISTER NOW" button. On the right side of the banner, there is a photograph of a diverse group of people in professional attire, smiling and clapping, suggesting a successful event or presentation.

ECS **240th ECS Meeting**
Oct 10-14, 2021, Orlando, Florida

**Register early and save
up to 20% on registration costs**

Early registration deadline Sep 13

REGISTER NOW

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

A Niozu^{1,2*}, Y Kumagai³, T Nishiyama^{1,2}, H Fukuzawa^{2,3}, K Motomura³,
M Bucher⁴, Y Ito³, T Takanashi³, K Asa^{1,2}, Y Sato^{1,2}, D You³, Y Li³,
T Ono³, E Kukk⁵, C Miron^{6,7}, L Neagu^{7,8}, C Callegari⁹, M Di Fraia⁹, G Rossi¹⁰,
D E Galli¹⁰, T Pincelli¹⁰, A Colombo¹⁰, T Kameshima¹¹, Y Joti¹¹, T Hatsui²,
S Owada², T Katayama¹¹, T Togashi¹¹, K Tono¹¹, M Yabashi², K Matsuda¹,
C Bostedt^{4,12,13}, K Nagaya^{1,2} and K Ueda^{2,3}

¹Division of Physics and Astronomy, Kyoto University, Kyoto 606-8501, Japan

²RIKEN SPring-8 Center, Sayo, Hyogo 679-5148, Japan

³Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

⁴Chemical Sciences and Engineering Division, Argonne National Laboratory,
9700 S. Cass Avenue, Argonne, IL 60439, USA

⁵Department of Physics and Astronomy, University of Turku 20014 Turku, Finland

⁶LIDYL, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette, France

⁷Extreme Light Infrastructure - Nuclear Physics (ELI-NP),

”Horia Hulubei” National Institute for Physics and Nuclear Engineering,

30 Reactorului Street, RO-077125 Măgurele, Jud. Ilfov, Romania

⁸National Institute for Laser, Plasma and Radiation Physics,

409 Atomistilor PO Box MG-36, 077125 Magurele, Jud. Ilfov, Romania

⁹Elettra - Sinchrotrone Trieste, 34149 Basovizza, Trieste, Italy

¹⁰Department of Physics, Università degli Studi di Milano, Via Celoria 16 - 20133 Milano, Italy

¹¹Japan Synchrotron Radiation Research Institute (JASRI), Sayo, Hyogo 679-5198, Japan

¹²Laboratory for Femtochemistry, Paul-Scherrer Institute, CH-5232 Villigen PSI, Switzerland

¹³Institute 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 corresponding to fcc{111}, {200}, {220} and hcp{101}

*E-mail: niozu.akinobu.85s@st.kyoto-u.ac.jp

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.

This study was supported by MEXT, JSPS KAKENHI, and IMRAM project.

References

- [1] Ishikawa T *et al* 2012 *Nat. Photon.* **6** 540
- [2] Mendez D *et al* 2016 *IUCrJ* **3** 420

