Crystallography

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Crystal evaluation for the determination of the Avogadro constant

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Introduction

The lattice spacing of a perfect silicon crystal is critical when determining the Avogadro constant by the X-ray crystal density (XRCD) method [1]. In the XRCD method, the Avogadro constant, N_A, is derived from the mean molar mass, M, the density, ρ, and the lattice spacing of the (220) plane, d_{220}, of a perfect silicon crystal using the following equation, $N_A = M/(8^{1/2}\rho d_{220}^3)$

The International Avogadro Coordination (IAC) project has performed various measurements using isotopically enriched silicon and has recently obtained the most accurate value, N_A=6.022 140 78(18)x10^{23} mol^{-1}[1], for a new definition of the kilogram.

Evaluation of homogeneity of silicon ingots as well as defects in silicon crystals is of great importance for the determination of N_A. Zhang et al. [2] have demonstrated a precision lattice measurement method using synchrotron radiation (SR) at KEK. In this paper, we present mapping results for the lattice spacing of the crystals 4.R1 and XINT[2], which were cut from the isotopically enriched crystal Avo28.

Principle of self-referenced lattice comparator

The principle and equations of the self-referenced lattice comparator (SRLC) method have been reported in Ref. [2]. This method uses a pair of quasi-simultaneously measured diffractions from the sample crystal. A slight change of the interval of two diffraction peaks was precisely measured to observe the lattice spacing variation in the crystal. The experiment was performed at the BL3C beamline of Photon Factory at KEK.

Mapping results and discussion

4.R1

Fig. 1 shows a map of the relative lattice spacing (the difference between pure white and black is 3×10^{-8}). Only a faint pattern of concentric ellipses is obtained. The areas indicated by the two circles correspond to the locations where the sample was supported by the pins; large deformations are observed in these areas due to its own weight. The 4.R1 is very homogeneous, even though a faint swirl pattern is still visible. These results demonstrate that this location in the Avo28 ingot has a very low strain, which suggests that the crystal is of sufficient quality to achieve an uncertainty of 3×10^{-9} in lattice spacing measurements.

XINT

The analyzer for the combined X-ray and optical interferometry technique for d-spacing determination, designated as XINT, was cut from isotopically enriched silicon Avo28. Fig. 2 shows a map of the relative lattice spacing. The brighter pixels in these plots correspond to larger lattice spacing (the difference between pure white and black is 6×10^{-8}). The XINT are homogeneous except for some regions where there are large differences in brightness, as shown in the figure. Black spots observed in the map of side A are highly localized in area and do not show anomalies at the corresponding positions on side B. These observations indicate that the crystal has no inherent strain that can deform large volumes (since otherwise they would be observed on both sides). These anomalies are separate from the rest of the crystal. The lattice spacing obtained by the combined optical and X-ray interferometry technique is the average value that excludes these points.

References

[1] B. Andreas et al., Phys. Rev. Lett. 106, 030801 (2011).
[2] X. Zhang et al., J Appl. Phys. 36, 188 (2003).
[3] H. Fujimoto et al., Metrologia 48, S55 (2011).

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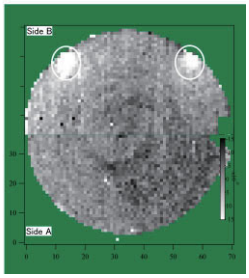

Fig. 1 Lattice spacing of 4.R1 on both sides of the disk.

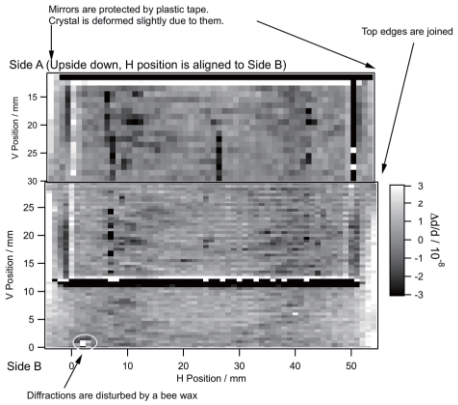

Fig. 2 Lattice spacing of the analyzer crystal of XINT.