Quality of silicon substrate and point defects
(9) Non-uniformity of lattice parameter and carbon concentration in Avogadro crystal

Radiation Research Center, Osaka Metropolitan Univ. [1] °N. Inoue[1], S. Kawamata[1] and S. Okuda[1]

シリコン結晶基板の品質と点欠陥 (9) アボガドロ結晶の炭素濃度分布と格子定数

大阪公立大放射線研究センター[1]　°井上直久[1], 川又修一[1], 奥田修一[1], E-mail: inouen@omu.ac.jp

In 2019, International System of Unit was redefined [1]. Kilogram prototype was practically replaced by the isotope enriched FZ Si sphere called Avogadro crystal. Lattice parameter (LP) of pure ^{28}Si was extrapolated from C-containing sample. The process requires the accurate [C] (C concentration) and conversion coefficient *k* from [C] to lattice shrink. Carbon is the largest source of error. In the last talk, we pointed out both include error [2]. There is another problem: Measured LP and [C] are average values over a certain volume in non-uniform sample. Relation between the averages is not equal to that between the true values.

(1) Here we demonstrate that highly sensitive and accurate measurement of local variation of LP provides the way to get accurate LP in pure crystal without using [C] and conversion coefficient. Windisch and Becker estimated the maximal and minimal values of LP in "natural" crystal with various [C] by the double crystal transmission X-ray topograph of vertically sectioned samples [3]. Δd/d in the highest [C] sample was $3.6\text{x}10^{-7}$. They attributed it to local variation of [C]. Measured [C] (average) was $2\text{x}10^{16}/\text{cm}^3$. The estimated [C] was between 0.05 and 2.5 x $[C]_{av}$. We performed similar analysis on synthetic quartz before [4].

Fujimoto, Waseda, Kuramoto and Fujii measured the LP variation in the Avogadro crystal using X-ray from SOR (synchrotron orbital radiation) by reflection topography [5, 6]. Measured [C] was $1\text{x}10^{15}/\text{cm}^3$ in the bottom of the crystal [7]. They got the LP variation to be $1.3\text{x}10^{-8}$. We examined their 1- dimensional map. The map showed nearly uniform LP with repeated sharp dips. We attribute them to nonuniform [C] due to segregation (remelt. and maximum growth rate). Rough estimate of minimal and maximal [C] (corresponding to maximal and minimal LP near remelt and highest growth rate) gives less than 1/10 and x5 of $[C]_{av}$ of $1\text{x}10^{15}/\text{cm}^3$. It is to be noted that [C] of less than $10^{14}/\text{cm}^3$ gives essentially LP_0 of C-free crystal within a range of error. Therefore, by measuring the local LP in the lowest [C] part, we can get LP_0. This does not need the ambiguous [C] and *k*. At present, local LP is obtained only relative to the average within the sample. If it is compared to the standard sample, the absolute number for "C-free" sample can be obtained.

(2) This shows the advantage and disadvantage of SIMS.

(a) Highly sensitive SIMS profiling will reveal the nonuniform [C] distribution and confirm the discussion from LP distribution and give insight to the segregation.

(b) SIMS usually gets [C] from narrow area with less sensitivity to IR. We have to confirm the averaging is correct enough.

(3) Research on point defects and grown-in defects will be developed after these examinations.

Comments by Dr. Waseda of AIST and Professor Ando of SOR are gratefully acknowledged.

[1] 9th ed. of the SI Brochure, BIPM (2019). [2] Inoue et al., JSAP 2022F, 20p-C206-8. [3] Windisch and Becker, Phil. Mag. A, 58, 435 (1988). [4] Takano and Inoue, J. Crystal. Soc. Japan, 13, 204 (1971). [5] Fujimoto, Waseda, Zhang, Metrologia, 48, S5 (2011). [6] Waseda, Fujimoto, Zhang, Kuramoto, Fujii, IEEE trans. instru. 66, 1304 (2017). [7] Zakel et al. Metrologia, 48, S14 (2011).