EFFECTS OF CRYSTALLITE SIZE AND SPECIMEN ROTATION ON TWO-DIMENSIONAL POWDER DIFFRACTION FIGURES

Shoki Ono, Daiki Hattan, Kento Wachi, and Takashi Ida
Advanced Ceramics Research Center, Nagoya Institute of Technology, Tajimi, Japan

We have reported the effects of finite crystallite numbers and rotation of powder specimen on the diffraction intensity data collected with scintillation counters [1, 2]. In this study, we have conducted statistical analysis about those effects upon the two-dimensional powder diffraction figures.

Quartz powder samples with the effective crystallite diameters of 7 μm, 12 μm and 23 μm [1] were filled into glass capillary tubes of 0.1 mm in diameter. Two-dimensional powder diffraction figures were collected with a flat two-dimensional detector (Dectris, PILATUS-100K) available on the beam line BL5S2 at Aichi Synchrotron Radiation Center in Japan. Twelve or six diffraction figures from stationary specimens after stepwise rotation were collected for each of the samples. The effective numbers of diffracting crystallites [1] were estimated for each of the diffraction figures by analysis of the integrated intensities along the quartz 101/011 Debye-Scherrer ring. The values of average and standard deviation of the numbers about 12 or 6 figures have formally been estimated at 0.16(9), 0.20(11) and 0.031(11) for the 7 μm, 12 μm and 23 μm samples, respectively.

On other measurement runs, the 23 μm powder specimen was continuously rotated at the rates adjusted to let the angular range of rotation during the exposure be 1.2° or 24°. The effective numbers of diffracting crystallites have been estimated at 0.05(2) and 1.0(2) for the angular range of 1.2° and 24°, respectively. The ratio is reasonably related to the assumption: the probability that a crystallite satisfies the diffraction condition is proportional to the angular range of specimen rotation.

[1] T. Ida, T. Goto and H. Hibino, *J. Appl. Cryst.* **42**, 597–606 (2009).
[2] T. Ida, *J. Appl. Cryst.* **44**, 911–920 (2011).