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Preferred Orientation Factor in Synchrotron Powder Diffractometry

Takashi Ida[1,2*] Yuki Togo[1], Hideto Funahashi[1] and Hisashi Hibino[1]
[1]ACRC, Nagoya Institute of Technology, Tajimi 305-0801, Japan
[2]AichiSR, Seto 489-0965, Japan

1 Introduction

The preferred orientation of crystallites is one of the important features in the texture of polycrystalline materials, particularly ferroelectric or ferromagnetic materials, for example.

On the other hand, the application of a preferred-orientation model is often required even in an ordinary analysis of powder diffraction data. The March-Dollase function [1] or spherical harmonics [2] is usually applied in most of the application software for Rietveld analysis. However, it should be emphasized that the above functions are intended to be used as the pole density profile function, and not the preferred orientation factor to correct the observed powder diffraction intensities.

There may be some confusion, because the preferred orientation factor is equivalent with the pole density function when the powder diffraction data are collected in the symmetric reflection mode, which is applied in the most popular geometry known as the Bragg-Brentano geometry for laboratory X-ray powder diffractometers. However, the mathematical formulas of preferred orientation factor are definitely different in the capillary transmission mode or the asymmetric reflection mode commonly applied in synchrotron powder diffraction measurements, and even in some of modern laboratory X-ray diffractometers with position-sensitive X-ray detectors. In this study, we have derived mathematical formulas and a practical method for numerical evaluation of the preferred orientation factors suitable for corrections of observed powder diffraction data measured in the capillary transmission and asymmetric reflection modes. The formula for the asymmetric reflection mode measurements have been applied to the analysis of incident-glancing-angle-scan powder diffraction intensity data.

2 Experiment

Finely ground (ca. 1 μm) powder of NaCl was uniaxially pressed and sintered at 585ºC for 2h to prepare a solid disk sample. The diffraction intensities of 17 reflections of the NaCl disk were recorded on varying the incident glancing angle on the BL-4B2 beamline at the Photon Factory in Tsukuba.

3 Results and Discussion

Figure 1 shows the observed diffraction intensities of the 200-reflection of the NaCl disk sample on variation of the incident-glancing-angle (Ω). The observed intensity profile are fitted by applying a model for the surface roughness [3] combined with a two-phase model comprising 0.75% of a phase with (100)-oriented March-Dollase model with the orientation parameter of $r = 0.22$, and 99.25% of randomly oriented phase. The observed intensity profile in Fig. 1 appears to be well reproduced by the applied model, but some of the profile of other reflections could not be reproduced by the same parameter about preferred orientation. It is suggested that the March-Dollase model is not suitable for simulating such relatively strong preferred orientation, easily introduced on sintering process.

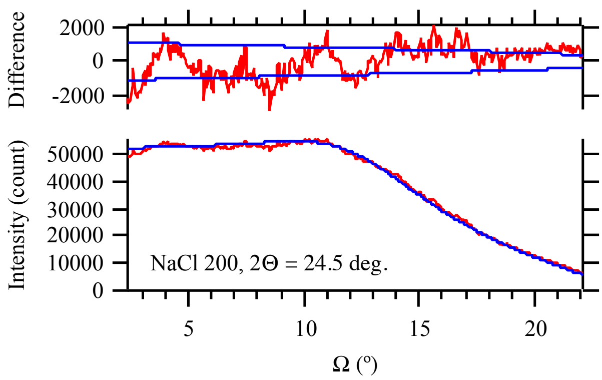

Fig. 1: The 200-reflection intensity profile observed on variation of the incident glancing angle (Ω).

References
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* ida.takshi@nitech.ac.jp