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Keywords: powder diffraction, structure determination, round robin

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Magnetic alignment to convert powder crystallites into a pseudo-single crystal

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Magnetic alignment of feeble magnetic crystals, including most of organic and inorganic materials, has been well known for long time, and the biaxial alignment has been utilized in materials science, for example, to improve superconducting quality.[1] This technique of biaxial alignment is also useful for the diffraction study. There are two types of diffraction methods, that is, single crystal method and powder method. Using the magnetic technique, we can offer the third method (pseudo-single crystal method) that enables to obtain single crystal diffractions from a powder sample.[2,3] Biaxial alignment of powder crystallites is achieved using a dynamic magnetic field, and the obtained sample (pseudo-single crystal) exhibits the diffraction pattern equivalent to the corresponding real single crystal. The advantages of this method are (1) no large crystal is needed so that it is useful for the analysis of nano- and micro-crystallites, (2) the sensitivity is greatly enhanced compared to the powder method because the diffraction points randomly dispersed for the powder pattern are condensed, and (3) it helps to resolve overlapping peaks encountered in the two-dimensional powder diffraction analysis.
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3D alignment of $LiCoPO_4$ microrods by modulated magnetic fields for X-ray single crystal analysis

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Crystallographic analysis of particles of nano to micrometer sizes has drawn increasing attention. However, the analysis is limited to powder analysis because of the size of the particles to be examined. If the single crystal analysis is allowed on a powder sample, the information obtained will greatly increased. In this present work, we demonstrate a magnetic technique that enables to convert a powder to a pseudo-single crystal and the resultant XRD pattern. We demonstrated (1) that the biaxial crystals including the orthorhombic, monoclinic, and triclinic systems are aligned 3-dimensionally if a modulated rotating magnetic field is applied to the suspension of these crystals. We have succeeded in alteration of an L-alanine powder to a pseudo-single crystal using a frequency-modulated elliptic magnetic field (2). In the present study, a LiCoPO4 powder was prepared by a modified hydrothermal method. The powder has square pole shape with ca. 2x2x20 mm^3. The magnetic alignment of the powder sample was carried out using two different types of modulated rotating magnetic field: amplitude-modulated and frequency-modulated magnetic fields. The powder suspended in a photo-curable resin precursor was subjected to the modulated rotating magnetic fields, and the alignment was fixed by photo-polymerization of the precursor to obtain a pseudo-single crystal. The obtained samples exhibited almost the same X-ray diffraction pattern that was comparable to the pattern of its equivalent single crystal, enabling the structure analysis of this compound.
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Keywords: pseudo-single crystal, modulated rotating magnetic field, $LiCoPO_4$ microrod

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Preparation of pseudo-single crystal of sucrose from powder by magnetic alignment

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Although the single-crystal X-ray analysis is a powerful means for the structure determination of crystals, a large single crystal is required for a successful analysis. In some cases, however, it is difficult to grow a large single crystal; only a powder sample is available. Powder analysis is also useful, but information obtained is limited. If the individual crystallites of a powder sample were all aligned three-dimensionally in a same manner, they would work as a pseudo-single crystal, giving X-ray diffraction comparable to the corresponding real single crystal. In fact, this is possible using magnetic alignment.(1,2) In this work, we report the preparation of a pseudo-single crystal of sucrose from its powder sample and discuss about the X-ray diffraction obtained from it. Large crystals of sucrose were pulverized to obtain a powder containing fine crystallites of 20 to 75 micrometer sizes. The crystallites were suspended in a UV-curable resin precursor and subjected to a modulated rotating magnetic field of 8 T, and then the achieved alignment was fixed by UV light irradiation. The obtained sample (a pseudo-single crystal) was subjected to the X-ray measurement. The obtained XRD pattern indicated that there are two types of crystal alignment in a magnetically aligned sample. This double alignment is regarded as a twin crystal. This observation is peculiar to the monoclinic system as expected by theoretical consideration.
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