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Determination of Crystal System from Microcrystalline Powder

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Determination of lattice constants is a crucial process in analyzing powder diffraction data, affecting the robustness of analyses in subsequent steps. A number of algorithms and software based on them to predict lattice constants from powder data have been reported. In this study, we propose a novel experimental approach to facilitate unambiguous determination of the crystal systems and resulting lattice constants from a microcrystalline powder sample. Efforts have been made for partial recovery of crystal anisotropy from a complete random orientation in powder in order to facilitate the analysis of powder data. Our approach makes use of magnetic orientation[1-3] of microcrystals occurring due to the diamagnetic anisotropy inherent to crystal. By application of a static/or rotating magnetic field, the easy/or hard magnetization axes of microcrystals undergo uniaxial alignment, giving rise to two different fiber diffraction patterns. These patterns reflect the crystal symmetry, enabling us to discriminate the crystal system. Crystals of known crystal system were pulverized and their suspensions were prepared. Each suspension was subjected to a static/or rotating magnetic field and the X-ray diffraction measurement was performed in situ to obtain two fiber diffraction patterns. It is evident that isotropic crystals only produce ring patterns for static and rotating measurement. On the other hand, biaxial crystals exhibit sharp diffraction spots in both fiber patterns. Furthermore, these fiber patterns exhibit layer lines in both patterns for the orthorhombic system, no layer lines for triclinic system, etc. In addition, overlapping of peaks in one-dimensional powder pattern can be resolved by indexing the spots in two dimensions of fiber patterns.

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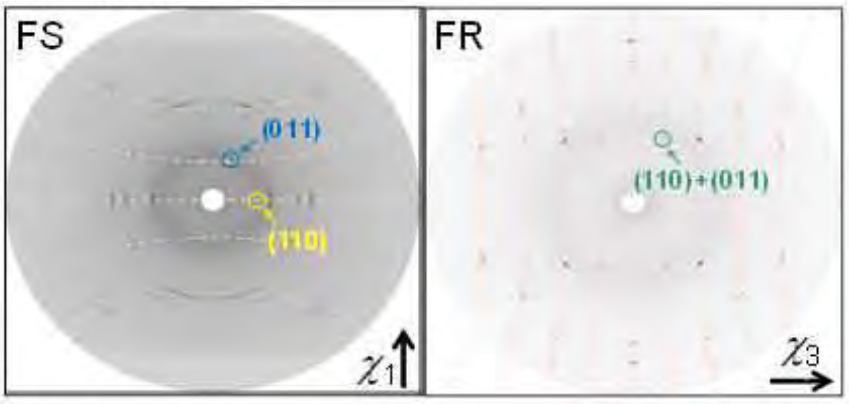

Figure 1 Fiber patterns obtained from microcrystalline powder of L-alanine (orthorhombic) measured under FS: static magnetic field and FR: rotating magnetic field. χ_1 (|| *c*-axis) and χ_3 (|| *b*-axis) indicate the easy and hard magnetization axes, respectively.

Keywords: crystal system prediction, microcrystalline powder, magnetic orientation