

Supplementary Materials.

S1. The Rietveld refinement for multi-synchrotron powder X-ray diffraction data.

The observation equation, S , is the same as normal Rietveld refinement which is single data analysis.

$$S = \sum_{i=1}^N w_i (Y_o(i) - Y_c(i))^2 \quad (1)$$

where, N is the number of data points, $Y_o(i)$ the observed intensity of data of i -th data points, $Y_c(i)$ the calculated intensity of data of i -th data points, w_i the weight of $Y_o(i)$. Here, number of data points of D_1 and D_2 are the ND_1 and ND_2 , observed intensities of D_1 and D_2 are the Y_oD_1 and Y_oD_2 . $Y_o(i)$ is

$$Y_o(1) \cdots Y_o(N) = Y_oD_1(1) \cdots Y_oD_1(ND_1), Y_oD_2(1) \cdots Y_oD_2(ND_2) \quad (2)$$

N is sum of ND_1 and ND_2 . By this treatment, two data are able to be treated as one data. In the refinement, the profile and background parameters are separately allowed for each data. As for the structure parameters, lattice constants, occupancy, fractional coordinates and thermal displacements, the same values are use with all the data.

S2. The Intensity extraction from multi-powder diffraction data

Observed Bragg intensities, $I_o(\mathbf{h})$, are extracted based on Rietveld refinement. There are D_1 and D_2 superimposed region in the present data. The intensities of the superimposed part are estimated by the sum of the intensities of D_1 and D_2 . Observed structure factors, $F_o(\mathbf{h})$, of not superimposed part in both D_1 and D_2 data are calculated from observed intensities as

$$|F_o(\mathbf{h})|^2 = I_{obs}(\mathbf{h}) / (S_i \cdot L \cdot P \cdot m) \quad (3)$$

where S_i is the scale factor of D_i data, L is the Lorentz factor, P is the polarization factors, m is the multiplicity. For superimposed part of D_1 and D_2 data, $|F_o(\mathbf{h})|$ are calculated using scale factor, S_i , and Bragg intensity, $I_{oi}(\mathbf{h})$, of each data as

$$|F_o(\mathbf{h})|^2 = \left(\sum_i^2 \frac{I_{oi}(\mathbf{h})}{2 \cdot S_i} \right) / (L \cdot P \cdot m) \quad (4)$$

Anomalous dispersion contribution are removed from structure factors (Bagautdinov et al., 1998) as

$$|F_o^{cor}(\mathbf{h})| = |F_o(\mathbf{h})| * |F_c^{cor}(\mathbf{h})| / |F_c(\mathbf{h})|$$

where $|F_c^{cor}(\mathbf{h})|$ is the calculated structure factors without anomalous dispersion, $|F_c(\mathbf{h})|$ is the calculated structure factors with anomalous dispersion.

The standard deviation of structure factors, $\sigma F_o(\mathbf{h})$, are normally express as

$$\sigma F_o(\mathbf{h}) = \frac{|F_o(\mathbf{h})|}{2} \left(\frac{\sigma S}{S} + \frac{\sigma I_o(\mathbf{h})}{I_o(\mathbf{h})} \right) \quad (5)$$

where σS is the standard deviation of scale factor determined by Rietveld refinement. In present study, $\sigma F_o(\mathbf{h})$ is estimated from the consideration of the structure factors extracted form two data as

$$\sigma F_o(\mathbf{h}) = \frac{|F_o(\mathbf{h})|}{2} \left(\frac{\sigma S^a}{S^a} + \frac{\sigma I_o^a(\mathbf{h})}{I_o^a(\mathbf{h})} \right) \quad (6)$$

where S^a and σS^a are the average value of scale factors of D₁ and D₂ data expressed as

$$S^a = (m \cdot S_1 + n \cdot S_2) / (m + n - j) \quad (7)$$

$$\sigma S^a = (m \cdot \sigma S_1 + n \cdot \sigma S_2) / (m + n - j) \quad (8)$$

where j is the number of superimposed reflections in D₁ and D₂ data, m is the number reflections of D₁ data, n is the number of reflections of D₂ data. Using the S^a , $I_o^a(\mathbf{h})$ and $\sigma I_o^a(\mathbf{h})$ are defined as

$$I_o^a(\mathbf{h}) = S^a \cdot L \cdot P \cdot m \cdot |F_o(\mathbf{h})|^2. \quad (9)$$

$$\sigma I_o^a(\mathbf{h}) = I_o^a(\mathbf{h})^{0.5}. \quad (10)$$

By these equations, two data are able to treat as one dataset.