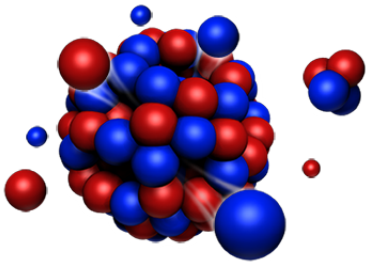

Contribution ID: **101** Type: **Poster**

Quantitative phase analysis of neutron powder diffraction results by using the direct-derivation method

The direct-derivation (DD) method has been recently proposed for quantitative phase analysis (QPA) of powder X-ray diffraction (XRD). It can be used to derive weight fractions of individual components in a mixture by using a simple equation, called the intensity-composition (IC) formula. The DD method requires two kinds of parameters which are the sum of observed powder diffraction intensities for each component, and the total scattering power per chemical formula weight obtained from the individual chemical formula unit. The DD method allows a sufficiently reliable QPA result by using limited information on chemical phases in a mixture than the Rietveld analysis. In this study, we tested the DD method for the QPA of neutron powder diffraction (NPD) results for several samples. The IC formula of the DD method is not suitable for NPD in principle, but our work has yielded relatively reliable results compared to XRD. The QPA results using the DD method in XRD and NPD will be presented. In addition, the criteria for the application of the DD method to the QPA of NPD will be discussed.

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Session Classification: Poster