A Rietveld refinement approach in structural study of bismuth zinc niobate cubic pyrochlores

Abstract

A brief introduction of Rietveld structural refinement and detailed procedure was discussed in this paper. High accuracy data is a prerequisite in structural study and therefore data are rendered from the state-of-art instruments, e.g. high resolution X-ray diffraction (XRD) and neutron diffraction (ND). The structural study of non-stoichiometric bismuth zinc niobate (BZN) pyrochlores was performed using General Structure Analysis System (GSAS); a comprehensive system for the refinement of structural models to both x-ray and neutron diffraction data. The stoichiometry calculated from the refinement was in excellence agreement to the phase diagram-determined stoichiometry. Powder neutron data were used to study oxygen sites as XRD data are insensitive to oxygen positions in the presence of heavy atoms such as Bi and Nb in the pyrochlore structure. The high R values and relatively long bond distance in A-O(1) indicated that displacement of A site cations were required in order to stable the structure, however, only preliminary steps and results were discussed at this stage; whilst, a more comprehensive displacement model would be addressed later.

Keyword: Rietveld refinement; Pyrochlore; X-ray Diffraction