

Structures and solid solution mechanisms of pyrochlore phases in the systems Bi₂O₃-ZnO-(Nb, Ta)₂O₅

Abstract

The crystal structures of two pyrochlore phases have been determined by Rietveld refinement of combined X-ray and neutron powder diffraction data. These are stoichiometric, Bi_{1.5}ZnTa_{1.5}O₇ and non-stoichiometric Bi_{1.56}Zn_{0.92}Nb_{1.44}O_{6.86}. In both structures, Zn is distributed over A- and B-sites; Bi and Zn are displaced off-centre, to different 96g A-site positions; of the three sets of oxygen positions, O(1) are full, O(2) contain vacancies and O(3) contain a small number of oxygen, again in both cases. Comparisons between these structures, those of related Sb analogues and literature reports are made.

Keyword: Ceramics; Solid state reaction; Crystal structure; Pyrochlore; X-ray and neutron diffractions.