Contribution ID: **11** Type: **Oral**

Thermal expansion behaviour of BPO4 studied by X-ray thermodiffractometry

This talk presents the crystal structure dynamics as a function of temperature of non-porous borophosphates. Much of the work published on these materials has focused on investigating the synthetic approaches as well as exploring their fascinating structural chemistry. Little has been reported about their thermal expansion behaviour. This thermoresponsive behaviour revealed their thermal stability while serving as a predictive measure of the effects of temperature on other materials properties and subsequent application. The thermal expansion behaviour of the non-porous cristobalite BPO4 phase is will be highlighted. BPO4, which crystallizes in the tetragonal lattice, showed a substantial anisotropic expansion in the lattice. This contrasting thermal expansion behaviour along the various axes of the material is related to the temperature variation of the inter-polyhedral angle between adjacent polyhedral in the crystal structure. This talk will also include total scattering data collected at the European Synchrotron Radiation Facility (ESRF), beamline ID22. This analysis is sensitive not only to the average (local-range) material structure but also the local distortions away from the average structure. Results will be reported relating to the total scattering investigation of the thermal expansion of the B-O and P-O bond-lengths in comparison with the values obtained by conventional X-ray diffraction measurements.

Summary

Primary authors: MOGODI, Mashikoane (University of Cape Town); BILLING, David (University of the Witwatersrand)

Presenter: MOGODI, Mashikoane (University of Cape Town)