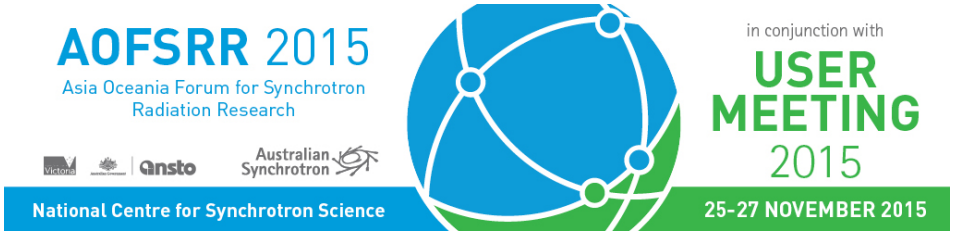

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Investigation of the Phase Transition of CuSb2O6 at High Temperatures by Synchrotron Powder Measurements

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The phase transition of CuSb2O6 has been described previously as a transition from tetragonal trirutile to distorted monoclinic trirutile structure. Cu2+ as a d9 system forms the square lattice oxide layer, which leads to a second order phase transition (Jahn-Teller distortion) [1]. The systematic reduction in symmetry would require the existence of an orthorhombic modification between the two modifications, surpressed in many structures. From synchrotron high temperature measurements, the phase transition in CuSb2O6 can be clearly observed and a possible two modification model (orthorhombic modification (Pnnm) and tetragonal modification (P42/mnm)) can be refined from 200 ℃ to 900℃ data. The direct phase transition from the monoclinic to the tetragonal modification is clearly surpressed over a large temperature range. The measurements show an unusual thermal behaviour. Some groups of diffraction peaks show an increase of the intensity as the temperature increases and others show a relative decrease of the intensity, but the thermal broadening decreases as the temperature increases. This is related to the ratio of the two high temperature modifications present at all temperature. The refined ratio of orthorhombic modification to tetragonal modification decreases from 200℃ to 900℃ but the phase transition is still not completed at 900℃. The refined lattice parameters indicate a normal thermal expansion of the unit cell, whereas the thermal broadening of the diffraction shows the opposite trend.

[1] A.V. Prokofiev, F. Ritter, W. Assmus, B.J. Gibson and R.K. Kremer, J. Cryst. Growth. 247, 457 (2003).

Keywords

Phase Transition, High Temperature, Solid State Chemistry, Synchrotron Powder Diffraction

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