Crystal structures of Th(Cu,Sn) compounds

FARZANA NASREEN, LUIS M. SANDOVAL, KARUNAKAR KHOTAPALLI, New Mexico State University, ALEXANDRE V. ANDREEV, HEINZ NAKOTTE, New Mexico State University — Powderized samples of Th(Cu,Sn) with nominal compositions of 1:1:1 and 1:2:2 were studied by neutron diffraction techniques using the NPD diffractometer at the Los Alamos Neutron Science Center. The structural analysis of the diffraction data was done using the Rietveld refinement package GSAS, which was developed at Los Alamos National Laboratory. For ThCuSn, assuming an orthorhombic structure with P21cn space group fits the neutron-diffraction data best. We still observed some unindexed reflection, which could be attributed to thorium dioxide as the second phase. The second sample was thought to be ThCu2Sn2, which crystallizes in the tetragonal P4/nmm phase. A careful analysis of the intensities revealed that not all of the Cu positions for this composition are occupied and that the actual composition of our second sample is closer to 1:1.5:2. A similar observation was reported for the magnetic analog UCu2Sn2.

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