

W0255

Skutterudites: Their Structural Response to Filling. B.C. Chakoumakos, Oak Ridge National Laboratory*, Oak Ridge, TN 37831-6393 USA.

The skutterudite structure, M_3Pn_{12} (cubic $Im\bar{3}$) where M = Group VIII transition metal, and Pn = pnictogen, can be filled to varying degree by up to one atom per formula unit of a lanthanide, actinide, alkaline earth, or thallium, $A_1M_3Pn_{12}$. A growing number of crystal structure refinements of filled skutterudites are being reported because of their interest as novel thermoelectric materials. Filled skutterudites possess high carrier mobility, high electrical conductivity, relatively high Seebeck coefficients, and glass-like thermal conductivity. The filling atom exhibits an anomalously large displacement parameter at room temperature due to its undersized filling of the atomic cage formed by the corner-linked octahedral framework of M_4Pn_{12} . Systematic changes in the framework structure correlate with the degree of filling. The Pn_4 ring becomes more regular as the filling fraction increases. Analysis of the temperature dependence of the atomic displacements identifies a significant temperature independent component for the filling atom ascribed to static disorder. The large amplitude rattling of the filling atom is linked to the dramatic decrease of the lattice contribution to the thermal conductivity.

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