PHYSICAL REVIEW B
covering condensed matter and materials physics
2009, Volume 59, Issue 1, p. 257-268

Phase transitions in defect chalcopyrite compounds under hydrostatic pressure

Ursaki V. V., Burlakov I. I., Tiginyanu I. M., Raptis Y. S. Anastassakis E. Anedda A.

https://doi.org/10.1103/PhysRevB.59.257

Abstract

Tetrahedrally bonded $AG_{a2}X_4$(A=Cd, Zn; X=S, Se) compounds crystallizing in defect chalcopyrite and defect famatinite structures have been studied by Raman spectroscopy under hydrostatic pressure. The pressure-induced changes in the Raman spectra of both ordered defect chalcopyrite and partially disordered defect famatinite structures were attributed to an order-disorder phase transition in the cation sublattice, which proved to occur in two stages, as predicted by Bernard and Zunger [Phys. Rev. B 37, 6835 (1988)]. The first stage of the transition was found to depend on the tetragonal distortion of the initial crystals. An irreversible disappearance of Raman signal at elevated pressures was observed and attributed to a phase transition from the adamantine structure to a high-symmetry rocksalt-type structure. The pressure of this transition in the compounds under consideration exhibits a dependence on bond ionicity and bond length. The structure of decompressed samples was explained on the basis of pressure dependence of potential barriers for the phase transition by using a configuration-coordinate model.