

Structural Characterization of the $\text{Cu}_2(\text{Se,Te})_3\text{-(Ga,In)}_2(\text{Se,Te})_3$ Semiconducting Systems

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Many contributions have been reported in the literature about the synthesis and characterization of chalcopyrite-related In- and Ga-rich ordered defect compounds of the ternary systems: Cu-In-Se, Cu-In-Te, Cu-Ga-Se and Cu-Ga-Te. Particular interest has been paid to the compounds that can be derived from the formula $\text{Cu}_{N-3}\text{In}_{N+1}\text{Se}_{2N}$, where $N=4, 5, 6, 7, 8$ and 9 , because some of these materials have already been used in important solar cell applications. The expectation is that $\text{Cu}(\text{In,Ga})\text{Se}_2$ will be the base of the solar modules of the future. It holds the best promise for the fabrication of high efficiency solar cells with long-term stability and a low production cost.

In this presentation, some the most important structural aspects of these materials will be discussed in the context of the crystal chemistry principles governing the formation of diamond-related tetrahedral structures, also called *adamantane structures*. Among others, the different structural models reported for some of the phases (including our own) will be presented. The difference in the dimensions of the unit cell (unit cell parameters and volume) among these materials is rationalized based on the fraction of cation vacancies and the amount of interacting donor-acceptor defect pairs $[\text{In}_{(\text{Cu})}^{2+}, 2\text{V}_{(\text{Cu})}^{-1}]$ per unit formula.

The structural studies carried out in several phases prepared by the Bridgman technique in a multi-zone vertical furnace were performed using powder diffraction data collected with a SIEMENS D-5005 diffractometer.