Diffraction Study of the Semiconducting $Cu_2(Se,Te)_3$-$(Ga,In)_2(Se,Te)_3$ 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 $Cu_{N-3}In_{N+1}Se_{2N}$, where N=4, 5, 6, 7, 8 and 9, because some of these materials have been already used in important solar cell applications. In the present work some the most important structural aspects of these materials will be discussed. Among others, the different structural models reported for some of the phases (including our own). The difference in the dimensions of the unit cell (unit cell parameters and volume) among these materials can be rationalized based on the fraction of cation vacancies and the amount of interacting donor-acceptor defect pairs [$In_{(Cu)}^{2+}$, $2V_{(Cu)}^{-1}$] 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.

This work was supported by grants from FONACIT (LAB-97000821) and CDCHT-ULA.

Keywords: powder x-ray diffraction, semiconductors, solar energy conversion