AB INITIO CALCULATIONS AND EXPERIMENTAL PROPERTIES OF CUALXGA1-XTE2 FOR PHOTOVOLTAICSOLAR CELLS

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Abstract

Nanostructured chalcopyrite CuAlxGa1-xTe2 (x =0.25, 0.50 and 0.75) has been prepared by ball milling of Cu, Al, Ga and Te precursors. Preliminary ab initio calculations of the main properties have been performed on the prototype chalcopyrite semiconductor CuAlGaTe2. The simulation method used is based on the density functional theory within the framework of pseudo-potentials and plane waves. Band structure calculation suggest that CuAlxGa1-xTe2 is a direct bandgap semiconductor having band gap = 1.35 eV. In the experimental part, X-ray diffraction analysis revealed the presence of (112), (220)/(204), (312)/(116) and (400) reflections for all the milled powders characteristic of the chalcopyrite structure. Shift in peaks towards higher value of 2□ is observed with the increase in Al composition. Lattice constants a and c are found to decrease with the increase in concentration of aluminium. With increasing Al content, it is found that the average crystallite size decreases and the bandgap energy increases from 1.34 eV to 1.51 eV. Compared with experimental data, calculated results by GGA–mBJ functional quantitatively agree with experimental data.

Keywords: CuAlGaTe2, photovoltaic, nanaoparticle, GGA-mBJ approach, Ab initio calculations, milling

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