Structure modifications in chalcopyrite semiconductors

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Abstract

The microstructure of epitaxial CuInS\textsubscript{2}, CuGaSe\textsubscript{2} and polycrystalline CuInS\textsubscript{2} films was studied by transmission electron microscopy. We found that the vapour-phase epitaxy of CuInS\textsubscript{2} below the transition temperature T\textsubscript{c} results in films with chalcopyrite and CuAu-like structures. The formation of CuAu-like ordered phases with the films is independent of the substrate orientation, whereas the amount of CuAu-like ordered Cu and In atoms can be influenced by the substrate orientation. The co-existence of chalcopyrite and CuAu-like ordering of the metal atoms was also found in polycrystalline CuInS\textsubscript{2} films prepared by sulphurization of Cu/In metal precursor at a temperature below T\textsubscript{c}. In contrast, vapour-phase epitaxy of CuGa_Se\textsubscript{2} below T\textsubscript{c} provides only films with the chalcopyrite structure. The experimental finding is in good agreement with the results of first-principle band-structure calculations.