Nanocomposites and nanomaterials

Grain boundaries in IV-VI nanocomposites: analysis of factors which may influence their composition during fabrication of nanocrystals

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Over the past decade a significant progress in the synthesis of narrow gap IV-VI (PbTe, SnTe, PbS and PbSe), nanocrystals demonstrated their high potential for higher efficiency thermoelectric converters. Recently, many methods have been developed to prepare IV-VI nanomaterials. Surface oxidation of resulting nanoparticles which is difficult to avoid is a common feature of almost all methods. Since there are no direct methods for determining the composition of boundaries in nanostructures, we applied different spectroscopic methods (TOF-SIMS, AES and X-ray diffraction) to evaluate and compare oxide compositions for a number of possible processes that may occur during nanocrystal fabrication of PbTe, SnTe, PbSe, SnSe, and of some their solid solutions. The obtained results demonstrate that the oxidation processes and the oxide composition are near the same at the substitution in the chalcogen sublattice (Te→Se), but they are strongly changed at the substitution in the metal sublattice (Pb→Sn). Under the same growing conditions, the grain boundaries will consist of a mixture of tin oxide and elemental chalcogen in SnTe and SnSe nanocomposites, and the ternary oxide ($PbTeO_3$ or $PbSeO_3$ forms the grain boundaries in PbTe and PbSe nanocomposites. For the solid solutions with the substitution in the metal sublattice, tin oxidation becomes a prevailing process, even in case of low tin content that is characteristic of solid solutions ($Pb_{0.8}Sn_{0.2}Te$ and $Pb_{0.93}Sn_{0.07}Se$). For the solid solutions with the substitution in the chalcogen sublattice ($PbSe_xTe_{1-x)}$, the oxide composition is directly associated with the composition of the solid solution itself.