Nanocomposites and nanomaterials

Spectra of the Elementary Excitations in the In_4Se_3 Crystals with Different Nanoinclusions

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Today the In_4Se_3 crystal has received considerable attention due to its high thermoelectric figure of merit, which has been newly discovered. In [1,2] it has been proposed that condenson states with a large size, which can exist in this In_4Se_3, have a key role in a reduction of thermal conductivity and increase of the Seebeck coefficients. We also discussed the possibility that the condenson-dependent thermoelectric properties could be tuned by incorporation of alloying elements into the crystal structure. Besides, we presented the direct observation of spherical nanoinclusions in $In_4Se_{2.6}$ and $In_4(Se_{0.95}Te_{0.05})_{2.6}$ by using transmission electron microscopy and discussed their structural and compositional properties. Therefore from this point of view, it is of interest to investigate the spectra of elementary excitations in the In_4Se_3 crystals with intrinsic nanostructural low dimensionality.

In this work, we carry out the simulations of the different types of nanoinclusions such as interstitial atoms, site substitution, vacancies and pair of defects in the In_4Se_3 crystal. First-principles investigations of the electronic structure and the spatial distribution of the electron density of In_4Se_3 with the Selenium deficiency and In excess and also the substitution impurities (Sn, Te) have been presented. Our obtained results explain the enhancement of the thermoelectric performance in the doped In_4Se_3 crystal.

1. *Y.S. Lim, M. Jeong, W.-S. Seo, J.-H. Lee, C.-H. Park, M. Sznajder, L. Yu.Kharkhalis et al.* Condenson state and its effects on thermoelectric properties in In_4Se_3 // J. Phys. D.: Appl. Phys.-2013.- **46.-**P. 275304 (5).
2. *M. Jeong, Y.S.Lim, W.-S.Seo, J.-H.Lee, Ch.-H.Park, M. Sznajder, L.Yu.Kharkhalis et al.* Condenson-related thermoelectric properties and formation of coherent nanoinclusions in Te-substituted In_4Se_3 / // Journ. of Materials Chemistry A.- 2013.- **1.-** P. 15342(6).