Electronic and Optical Properties of Heterostructures Based on Indium Chalcogenides

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The indium chalcogenides keep attracting an increasing attention because of their wide applications in the optoelectronics devices development as a highly sensitive dynamic and static strain sensors. In this context, the semiconductor compounds of the In-Se system and their solid solutions are used for the production of the photosensitive elements on the basis of the homo- and heterojunctions, which have been obtained by van der Waals epitaxy method and laser restructuring [1,2]. The formation of the In_4Se_3/In_4Te_3 and β-InSe/In_4Se_3 heterostructures leads to widening of the spectral sensitivity range of the photoelements. It is established that these elements are sensitive within the range of 1.0-2.0 μm and thus are successfully used as infrared detectors and filters.

To contribute to the understanding of the spectral characteristics formation of the photosensitive devices, we study the electronic structure and optical properties of the different type heterostructures built upon In_4Se_3, In_4Te_3 and β-InSe crystalline semiconductors. Considered choose of the crystals is made by virtue to obtain the stable heterostructures with the perfect interfaces. In this connection it should be noted that while In_4Se_3 and In_4Te_3 orthorhombic crystals (D_{2h}^{12} space symmetry) are isostructural materials and lattice mismatching between constituent materials of heterostructures are small (~ 2%), the In_4Se_3 and β-InSe (D_{6h}^{4}) layered crystals have completely different lattice types and form the strained heterostructures [3].

In this work, we present first-principles investigations of the electronic structure and optical properties of the heterostructures of $(In_4Se_3)_m/(In_4Te_3)_n$ and β-InSe/In_4Se_3 type. The band spectrum, the spatial distribution of the electron density, real and imaginary parts of the dielectric function, the absorption coefficient for different polarizations along crystal axes were calculated. The evolution of the changes in both energy spectrum and optical functions of the heterostructures in comparison with the bulk crystals had been analyzed. It is shown that the forbidden energy gap increase and consequently the widening of the spectral sensitivity range take place with the increase of the heterostructures thickness. The strain-induced electronic structure changes in the β-InSe/In_4Se_3 heterostructures have been analyzed well. Our calculations suggest a good agreement with results of known experimental investigations. It points out the possibility of the forming of the stable heterostructures on the base of the indium chalcogenides, which can ensure essential photosensitivity in the near and middle infrared region.

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