Abstract

Topological properties of selected IV-VI semiconductor nanostructures

In this thesis, the results of a research on the topological properties of selected nanostructures made of IV-VI materials are presented. Some binary and ternary IV-VI crystals have an inverted band gap and belong to the class of topological crystalline insulators (TCI). As a result of the non-trivial topology of electronic band states, they have an even number of gapless states with Dirac cone dispersion on their surfaces. Remarkable experimental achievements obtained for SnTe and its ternary crystalline solid solutions, such as (Pb,Sn)Te/Se, confirmed the existence of non-trivial surface states. They have stimulated extensive research efforts not only on bulk crystals but also on nanostructures and defects in recent years. Here the results of theoretical studies on nanostructures with defects in the form of (111) oriented twin planes (TP) are discussed. The discussion focuses on three different types of nanostructures. These are super-lattices, thin films and nanowires. In the case of films and wires, the obtained results are compared with the properties of similar structures without defects. The analysis of the results reveals that TPs can be treated as two-dimensional topological structures belonging to the TCI class which are protected by the (111) mirror symmetry. The value of the topological invariant - the mirror Chern number - depends on the type of twinning and is equal to 1 for an anionic TP and to 2 for cationic one. It is also shown that at the one-dimensional edges of these structures, the expected number of topologically protected non-trivial boundary states appears. However, in sufficiently thin film with surface orientation (111) having a TP defect in the middle, the topological effect is destroyed by a hybridization of the electronic surface states with the states located on the defect. The protected edge states still appear and show the quantum spin Hall effect, that is only due to the existence of the same \mathbb{Z}_2 invariant that defines the topology of non-defective structures. In the second part of the thesis, the topological properties of a pentagonal SnTe quantum wire are described. Its cross-section shape comes out from the existence of five TPs extending radially from the center. The wire has two non-trivial electronic states: one located in its center and another one located on its five edges. It is established that their presence is related to the topological properties of TPs. The result has been compared with the properties of a wire with a square cross-section, where the edge states are of a different nature; these are topological states of the second order - hinge states. It is shown that they are not as robust against hybridization as the edge states in wires with an odd number of edges.

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