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REVIEW OF THE DOCTORAL DISSERTATION

of Mr. Saeed Samadi Bahnemiri, M.Sc.,

entitled *Topological properties of selected IV-VI semiconductor nanostructures*

Mr. Saeed Samadi Bahnemiri, M.Sc., prepared his doctoral dissertation entitled "*Topological properties of selected IV-VI semiconductor nanostructures"* under the supervision of Prof. dr hab. Ryszard Buczko *[professor, Ph.D., postdoctoral degree holder]* at the Institute of Physics of the Polish Academy of Sciences in Warsaw. The doctoral dissertation is written in English and contains 6 chapters, including an Introduction, Summary, and Supplement. The paper also provides an Abstract in Polish and English. The author's original results, some of which were published this year in Physical Review B (reference in dissertation no. 133), are described in Chapter 5. The entire work has 133 pages and contains 151 references.

The subject of the dissertation is ambitious and highly relevant. The Ph.D. candidate chose to investigate the topological properties of selected nanostructures based on IV-VI semiconductors, categorized as topological crystalline insulators (TCIs) exhibiting gapless Dirac surface states. In this study, the candidate focused on the role of twinning planes (TP), which are regular adhesions or defects in the crystal structure within the (111) plane, and on the topological properties of crystal topological insulators. Three types of nanostructures were selected for analysis: superlattices, thin films, and nanowires based on SnTe. To characterize the topological attributes of these nanostructures, the Ph.D. candidate needed to master numerical methods enabling band structure calculations, developed within Professor Buczko's team, and knowledge of the topological properties of matter, including the methodology for calculating topological invariants.

Chapter 2 of the dissertation contains an introduction to the topological properties of matter. The author presents the basic information necessary to characterize the electronic band structure in terms of its topological properties. Thus, the concept of adiabatic evolution of the cyclic and geometric phase of the wave function, commonly known as the Berry phase, is introduced. This concept is then used to describe the Blochian evolution of electron wave functions in a solid. The Ph.D. candidate shows the relationship between the Berry curvature and the Chern number and introduces the concept of "bulk-boundary correspondence". In Section 2.6, the Ph.D. candidate presents the most important theoretical models describing selected systems with non-trivial topological properties. The historical context is initiated with the first system demonstrating topological properties, specifically one in which the complete quantum Hall effect is realized. The author highlights the TKNN theory, which connects the Chern number with quantum Hall conductivity. Subsequently, the candidate describes the so-called Chern insulators, focusing on the Qi-Wu-Zhang (QWZ) model. Using this model as an example, the author presents calculations of the Berry curvature, Chern number, Hall conductivity, and edge states. Next,

the Author discusses topological insulators with preserved symmetry with respect to time reversal on the example of the Bernevig-Hughes-Zhang (BHZ) model. This subsection also introduces the topological invariant Z_2 and methods for its determination.

Chapter 3 is an introduction to the physics of crystalline topological insulators, a class of topological materials introduced by Liang Fu in 2011. These materials exhibit topological properties in the band structure closely linked to the specific symmetry of the material's crystalline point group, which results in the appropriate symmetry of the atomic arrangement on the crystal surface. These are materials with protected mirror symmetry. The author defines the so-called mirror Chern numbers and proceeds to describe the band structure of crystalline topological insulators IV-VI with the general formula $Pb_{x-1}Sn_xTe$. Using the four-band Hamiltonian $\boldsymbol{k \cdot p}$ as an example, describing IV-VI semiconductors in the vicinity of the L point of the Brillouin zone and employing first principles calculations, the Ph.D. candidate illustrates the differences in the band structure of SnTe and PbTe. This distinction points to the existence of an inverted band structure in SnTe and the existence of a crystalline topological insulator phase, while PbTe is a trivial insulator. Then, the TCI surface states are characterized for the (111) and (001) surfaces. Section 3.2.3 provides an overview of the topological phases of SnTe thin films. Chapter 3.3 briefly mentions the impact of disturbances on TCI surface states, with a focus on structural distortions, magnetic admixtures, and mechanical stresses. In Chapter 3.4, the Ph.D. candidate introduces the concept of higher-order topological insulators (HOTIs) and suggests the feasibility of implementing HOTIs in SnTe structures.

Chapter 4 provides a description of the methods used by the Ph.D. candidate, including an introduction to the tight-binding model, the Slater-Koster formalism, and a brief description of the iterative method based on Green's functions. Towards the end of Section 4.1, the author provides a brief explanation of the assumptions of the tight binding model used in the Ph.D. candidate's calculations. Here the author writes *"our TB code"*. I would like the author to clarify the meaning of this statement during the defense. Did the Ph.D. candidate only work on the code developed by Professor Buczko and colleagues, or did he developed it to some extent?

Chapter 5 presents the original results obtained by the Ph.D. candidate, organized into 4 subchapters that delve into superlattices, thin films, and nanowires constructed from IV-VI semiconductors featuring structural defects in the form of twinning. At this point, I must emphasize the author's meticulous analysis of numerous systems, reflecting a high level of diligence This extensive analysis will certainly result in future publications involving the Ph.D. candidate, as well as prompt a broader literature discussion of the results obtained by Professor Buczko's team.
In Section 5.1, the candidate explores superlattices based on SnTe with twinning in the (111) plane. Twinning occurs in two planes within the supercell, where each plane constitutes a local plane of mirror symmetry. The studied superlattices can be categorized into three groups based on the layer – cationic or anionic – experiencing defects. Consequently, cation-cation (cat-cat) and anion-anion (an-an~~)~~ superlattices belonging to the $P6_3/mmc$ spatial symmetry group and mixed cation-anion (cat-an) superlattices with the $P\bar{6}m2$ spatial symmetry group were considered. The author first considered the topological properties of the band superlattice structure with different positions of the planes on which twinning occurs. In Chapter 5.1.2, band structures for a superlattice with a thickness of 200 atomic layers are presented, plotted along the paths *Γ-M-K-Γ* and *Γ-A-L-M-Γ* (additionally, band structures for the *A-L-H-A* path are available in Appendix A*)*. The obtained structures show that the states located on the twin planes are incorporated into the energy gap area. Topological invariants Z_2 were also determined (for TSL with inversion symmetry – using the method proposed by Fu and Kane; for TSL without inversion symmetry – using the method proposed by Fukui), and mirror Chern numbers using the Fukui method. Thus, the mirror Chern numbers for

the *ΓMK* plane are: 4 for superlattices with twinning planes in the cation-cation layers; 2 in the anion-anion layers; and 3 for twinning in the cation-anion layers. On the *ALH* plane, the Chern numbers are 0 for TSL of the cation-cation and anion-anion types, while for the cation-anion TSL, it is 1. For the $(1\bar{1}0)$ mirror plane corresponding to the *ALΓM* plane, the mirror Chern numbers are 2 for each TSL type. This analysis establishes that the selected three TSL types (cat-cat, an-an and cat-an) belong to different topological classes based on the mirror Chern numbers for the *ΓMK* plane. Section 5.1.3 offers a detailed analysis of the Berry curvature's behavior and the results of its local integration around high symmetry points, which confirm the results of the previously obtained mirror Chern numbers. In Section 5.1.4, surface states for superlattices with twinning are discussed. The analysis used the recursive method of Green's function to the tight-binding Hamiltonian describing a semi-infinite super-lattice ending with a surface with one of two orientations perpendicular to the crystal growth axis, i.e. $(1\bar{1}0)$ and $(11\bar{2})$. The presented spectral functions for the $(1\bar{1}0)$ surface in all types of analyzed superlattices show two energetically separated Dirac points in $\overline{M}$ and two secondary Dirac points in the middle of the gap, shifted relative to the $\overline{M}$ point towards the $\overline{\Gamma}$ point. Additionally, the cat-cat TSL spectrum shows a similar structure around the $\overline{\Gamma}$ point, with secondary Dirac points in the gap, shifted relative to $\overline{\Gamma}$ in the $\overline{M}$ direction, while the spectrum of an-an TSL shows surface states with a gap at the $\overline{\Gamma}$ point. In the case of the cat-an TSL lattice, however, there are single topologically protected Dirac points at $\overline{\Gamma}$ and $\overline{A}$ points. For the $(11\bar{2})$ surface, the obtained surface states along $\overline{M}$-$\overline{\Gamma}$ are qualitatively similar to those for the $(1\bar{1}0)$ surface. Furthermore, for the surface $(11\bar{2})$ along the $\overline{\Gamma}$-$\overline{A}$ line, additional Dirac states emerge (Dirac crossing) due to the unbroken mirror symmetry $(1\bar{1}0)$ resulting from the termination on the $(11\bar{2})$ surface. The Ph.D. candidate then provides an argument for the existence of calculated gapless surface states, based on the calculated Berry curvatures.

In Chapter 5.2, the Ph.D. candidate performs an analysis similar to that in Chapter 5.1.1, but for a two-dimensional layer with global mirror symmetry with respect to (111) with one twinned surface (cationic and anionic) with a thickness that excludes hybridization between the surface states and states located on the twinning. The candidate examines both the situation when the surface states are not disturbed (four surface Dirac cones can be observed – one at $\overline{\Gamma}$ point and 3 at $\overline{M}$ point) and when the disturbance (here *valley-mixing*) opens a break in the surface states. This analysis provides a more comprehensive understanding of how twinning influences the band structure of two-dimensional nanostructures.

Chapter 5.3 contains a very valuable discussion on the implementation of the spin Hall effect in a thin layer oriented in the direction of growth (111) and containing crystalline defects in the form of twinning. For IV-VI semiconductors that are crystalline topological insulators, the theoretical prediction of the quantum spin Hall effect phase has been made for layers growing in the [111] direction within a certain range of layer thicknesses. This prediction is related to the hybridization of surface states, leading to the emergence of the 2D TI phase, with a topological invariant Z_2, protected by symmetry with respect to time reversal. The quantum spin Hall effect phase is linked to the fact that the 4 L points projected onto the two-dimensional Brillouin zone are not equivalent. Therefore, if the energy structures in the three $\overline{M}$ projections are symmetric, the energy structure in the fourth projection at $\overline{\Gamma}$ point is different, enabling the inversion of the band structure at an odd number of points in the two-dimensional Brillouin zone. The Author of the dissertation analyzed the oscillations of the energy gap width and topological invariants as a function of the number of atomic layers constituting the examined thin layers. In the absence of defects in the crystallographic structure, it is established that the insulator state with the quantum spin Hall effect is observed for both even and odd numbers of atomic layers. The Ph.D. candidate examined scenarios involving twinning in the middle of structures

with an odd number of atomic layers, calculating the Z_2 invariant using the Fu-Kane method and the mirror Chern number. Four cases were analyzed: a layer terminated with an anionic plane with twinning in the anionic layer and with twinning in the cationic layer, and a layer terminated with a cationic plane with twinning in the cationic layer and with twinning in the anionic layer. The candidate notes that in layers with cationic twinning, band inversion occurs for thicknesses between 15 and 29 monolayers, 33 monolayers, and for thicknesses between 51 and 59 monolayers. For anionic twinning, band inversion occurs for layers with thicknesses from 21 to 27 monolayers and for layers with a thickness of 31 and 57 monolayers. For thin films with thicknesses of 9, 21, 41, and 57 monolayers, the Ph.D. candidate presents Berry curvatures for both anionic and cationic twinning structures and discusses their topological properties. Then, in Section 5.3.2, the author uses the iterative Green's function method to calculate edge spectral functions for the studied systems. Here, the author considers a layer terminated with a cationic surface with a cationic twinning type and a layer terminated with an anionic surface with an anionic twinning type. The Ph.D. candidate determined the bulk and edge states for the thin layer (111), composed of 13 and 21 monolayers, and the spin density of states for the one-dimensional Brillouin zone for the edges $[11\bar{2}]$. Gapless edge states at the $\bar{\Gamma}$ point have been found with a topological invariant Z_2 equal to 1 and with a mirror Chern number equal to +1 for the structure terminated with an anionic layer and -1 for the structure terminated with a cationic layer.

In Chapter 5.4, the author considers nanowires made of a crystalline topological insulator growing in two directions: in the [011] direction with a pentagonal cross-section and in the [001] direction with a square cross-section.

First, the Ph.D. candidate analyzes the band structure of the pentagonal SnTe nanowire (subsection 5.4.1.2), which has both surface states and topological core states (TCS) typical of nanowires, as well as the so-called hinge states. The author discusses in detail the coexistence of these states, illustrating the core states, hinge states, and surface states of the crystalline topological insulator. The candidate draws attention to, among other things, the fact that hinge states hybridize with each other and with surface states. Later in the chapter, Mr. Samadi Bahnemiri decomposes the Hamiltonian written in the subspaces of states of the C_5 symmetry operator and shows the existence of gapless core states with the opposite chirality to the hinge states. It should be noted here that, according to the results obtained by the candidate, topologically non-trivial states are obtained only for the nanowire with cationic twinning, while in the nanowire with anionic twinning, gapless modes are absent. A pentagonal nanowire made of the $Pb_{0,6}Sn_{0,4}Se$ alloy behaves quite similarly, where for cationic twinning, the author found topological core states and topological edge states, while in the case of anionic twinning, anti-crossing and trivial behavior of surface states and core states appear. In subsection 5.4.1.4, the candidate analyzes a SnTe nanowire whose side walls are made of $(21\bar{1})$ planes. In this case, the twinning planes form a plane normal to the $(21\bar{1})$ plane and cut each of the five side walls of the nanowire in half. The analysis shows that the single topological state of the core is independent of the topological properties of individual twinnings and is insensitive to the location of the twinning planes as long as the C_5 symmetry is maintained. In sections 5.4.1.5 and 5.4.1.6, the Ph.D. candidate examines in detail the behavior of hinge states and core states. At the end of Chapter 5, the author analyzes hinge states and the effect of their hybridization for a nanowire with a square cross-section.

In Chapters 5.2.3, 5.4.1.2 and 5.4.1.6, the Ph.D. candidate emphasizes the role of Mr. Rafał Rechciński in analyses performed. Since the authors of publication [133] are both Mr. Saeed Samadi Bahnemiri and Mr. Rafał Rechciński, and the publication is the only published work of the Ph.D. candidate that I have managed to find, I would like the candidate to explain

in detail his and Mr. Rechciński's contribution to the publication during his defense. I would like to know whether the statements: "*Rafał Rechciński (...) has explorer and implemented two metodologie in this Research [133]*", and "*analysis conducted by Rafał Rechciński*" mean that Mr. Rechciński only analyzed the results and the Ph.D. candidate was responsible for the numerical calculations, or do these statements mean that Mr. Rechciński was responsible for all the results obtained (calculations and analysis).

To sum up the entire doctoral dissertation, I believe that the subject of the work covers very interesting aspects regarding the topological properties of nanostructures based on crystalline topological insulators. The work contains many original findings. The author examined in great detail the role of twinning on the topological properties of SnTe superlattices and nanowires. Particularly commendable are the results in Chapter 5.3, where the Ph.D. candidate examines SnTe thin films of varying thicknesses and twinning types in terms of the implementation of the quantum spin topological insulator phase. Chapter 5.4 also stands out, as the Ph.D. candidate investigates the impact of twinning on the topological properties of nanowires, highlighting that in the case of wires with a pentagonal cross-section, topologically non-trivial states emerge only when the topological phase of the material from which the wire is made is topologically non-trivial and when the five twinned planes forming the nanowire are of the cationic type. The doctoral dissertation carried out a series of calculations to obtain full information about the band structure, topological properties, and the role of twinning in the studied nanostructures. The entire work is written in a clear and logically coherent manner. There are some linguistic shortcomings that I must note as a reviewer, but they do not affect the readability and comprehension of the content. Additionally, the dissertation's graphic design was prepared very carefully, which is worth emphasizing due to the vast amount of data and charts.

Due to the above, I have no doubt that the doctoral dissertation submitted to me for review meets the statutory requirements for a doctoral dissertation, and I recommend that Saeed Samadi Bahnemiri, M.Sc., be admitted to further stages of the procedure for the awarding of the doctoral degree.

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