MUNI

Annex No. 10 to the MU Directive on Habilitation Procedures and Professor Appointment Procedures

HABILITATION THESIS REVIEWER'S REPORT

Masaryk University	
Applicant	Mgr. Ondřej Caha, Ph.D.
Habilitation thesis	Thin films of topological insulators
Reviewer	Prof. Dr. Hab. Tomasz Story
Reviewer's home unit, institution	Institute of Physics, Polish Academy of Sciences, Warsaw (Poland)

Habilitation thesis of Ondrej Caha concerns experimental studies of thin films of topological insulators with the use of X-ray diffraction and X-ray spectroscopy techniques as well as electron photoemission spectroscopy methods, both in laboratory and in synchrotron facility environment.

Research on topological materials constitutes nowadays a vast and rapidly developing field of condensed matter and materials physics covering electronic systems, like topological insulators, topological Dirac or Weyl semimetals or topological superconductors, with many topological concepts expanding towards very different physical fields, like, e.g., topological photonics. The progress in verification of new theoretical or applicational concepts critically depends on developing growth methods and thorough experimental studies of structural and electronic properties of new materials in their various forms. Topological thin films and layered heterostructures are among the most important classes of such materials. Therefore, the subject of O. Caha's habilitation thesis should be considered as a very timely, while the research reported as internationally recognized.

Candidate proved his status as a world-class specialist in developing and application of various X-ray diffraction and spectroscopy experimental tools to study new electronic materials, in both the form of bulk crystals and epitaxial thin films. Importantly, it was done in very close collaboration with leading European laboratories in the field: Johannes Kepler University in Linz (Professors Günther Bauer and Gunther Springholz) and Helmholtz Zentrum Berlin (Professor Oliver Rader). It provided O. Caha regular access to new materials and advanced synchrotron experimental techniques and resulted in important scientific observations identifying the real space arrangement of constituent atoms in topological films. For several topological layered hetrostructures, in particular magnetic ones, it constituted an important step towards understanding the electronic properties of these new electronic materials.

Habilitation thesis is composed of introduction (chapter 1), two useful and well written chapters with author's presentation of the field of topological insulators (chapter 2) and a description of experimental methods applied in the studies of thin films of topological materials (chapter 3). Chapter 4 contains reprints of nine selected papers published in the

period 2013 - 2021 with candidate's important, individual contributions. Conclusions and outlook are presented in chapter 5.

The selected papers cover three main classes of topological materials, in the form of thin films, studied by O. Caha.

1. Bi_2Te_3 – Bi_2Se_3 topological insulators of Z_2 class.

The important result of three selected publications (Crystal Growth and Design 2013, J. Appl. Crystallography 2014, and Phys, Rev. B 2017) concerns the structural analysis of epitaxial films of Bi-Te topological materials system grown by molecular beam epitaxy (MBE) method in a broad stoichiometry regimes: from BiTe to Bi_2Te_3 topological insulator. The XRD data analysis, with new methodology developed by O. Caha for X-ray diffraction on random multilayer stacks, is correlated with the studies of electronic structure and optical properties.

2. Magnetically doped Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 topological insulators.

In four publications co-authored by O. Caha (Nat. Commun. 2016, New J. Phys. 2015, Nature 2019, and Adv. Mat. 2021) authors undertake the important technological and experimental task of developing new ferromagnetic topological insulator material constituting a platform for important effects foreseen, like quantum anomalous Hall effect with quantized electric conductivity. The X-ray diffraction and spectroscopy (EXAFS) as well transmission electron microscopy (TEM) data allowed for identification of true atomic arrangement in Mn doped Bi_2Te_3 - the task of O. Caha in these collaboration consortia. Mn doped Bi_2Te_3 turned out to form a multilayer heterostructure build of standard quintuple Bi_2Te_3 and magnetic septuple $MnBi_2Te_4$ layers. The temperature dependence of electronic structure (photoemission - ARPES) and magnetization revealed the correlation between magnetic properties and opening of energy gap in the spectrum of topological states.

3. Topological crystalline insulators: $Pb_{1-x}Sn_xTe$ and $Pb_{1-x}Sn_xSe$ substitutional alloys.

Two selected publications (Nat. Commun. 2017 and Adv. Mat. 2017) are devoted to topological crystalline insulators (TCI) - the class of topological materials relying on certain crystalline symmetries. Two important effects induced by Bi doping of thin epitaxial films were discovered. (1) Crystal lattice deformation induced transition from TCI (even number of band inversion at 4 L-points of the Brillouin zone) to Z_2 topological insulator (odd number of inversions) in $Pb_{1-x}Sn_xSe$. X-ray analysis of thin films by O. Caha confirmed the presence of such lattice distortion. (2) A discovery of giant Rashba spin splitting of surface electronic states in TCI $Pb_{1-x}Sn_xTe$ (111) layers.

Publication record of O. Caha is very good with more than 80 papers published mostly in prestigious international journals, like Nature (1 publication), Nature Communications (3), Physical Review Letters (2), Physlcal Review B (10) and Advanced Materials (2), with total of about 960 citations. Inspection of a complete list of publications (provided in chapter 6) reveals that O. Caha, apart from the field of topological materials, contributed to experimental

studies of structural and electronic properties of many semiconductor materials (III-V compounds, GaN, Si, Si-Ge alloys or ferromagnetic (Ga,Mn)As layers) and other systems.

Reviewer's questions for the habilitation thesis defence

1. Family of IV-VI compound semiconductors built of cations (Pb, Sn, Ge) and anions (Te, Se, S) hosts topological crystalline insulators (TCI), like rock-salt SnTe crystals. However, apart from cubic materials there also are bulk IV-VI crystals of lower (rhombohedral or orthorhombic symmetry), like GeTe, SnTe or SnSe. As crystalline (110) mirror-plane symmetry warrants protection of TCI topological states one may wonder whether these non-cublc distortions observed in bulk crystals can drive transition from the TCI to trivial or to other, topologically distinct class, thus influencing the spectrum of (001) or (111) surface electronic topological states? Can crystal lattice or thermal mismatch induced strain be used to engineered such topological transition in epitaxial topological films?
2. Many topological materials, e.g. $Bi_{1-x}Sb_x$, $(Bi_{1-x}Sb_x)_2Te_3$ or $Pb_{1-x}Sn_xTe$, are (substitutional) solid solutions of elements or compounds and, therefore, inherently exhibit local chemical and electronic disorder. Are there any X-ray diffraction or spectroscopy observations that support the validity of, so called, virtual crystal approximation, frequently used physical model in which local translational symmetry is restored in alloys with the use of effective composition-weighted electronic potentials?

Conclusion

The habilitation thesis entitled "Thin films of topological insulators" by Ondřej Caha fulfils requirements expected of a habilitation thesis in the field of Condensed Matter Physics.

Date: December 15th, 2023. Signature: