Thickness-dependent gap energies in thin layers of $HfTe_5$

Christopher Belke[1*], Sonja Locmelis[2*], Lars Thole[1*], Lina Bockhorn[1*], Hennrik Schmidt[1], Peter Behrens[2*] and Rolf J. Haug[1*]

1 Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

2 Institut für Anorganische Chemie, Leibniz Universität Hannover, D-30167 Hannover, Germany

** Laboratorium für Nano- und Quantenengineering, Schneiderberg 39, D-30167 Hannover, Germany*

Hafnium pentatelluride ($HfTe_5$) is a layered two-dimensional material with various exotic properties. One of these properties is a unique resistivity anomaly, which can be explained by a change in the band structure. Also, it is predicted that $HfTe_5$ is a topological insulator (TI) with a transition between weak to strong TI. Moreover, one of the most prominent predicted features of $HfTe_5$ is that its single layer is a quantum spin Hall insulator. To observe the quantum spin Hall effect at room temperature a large bandgap is essential. In bulk $HfTe_5$ the band gap has been experimentally determined to be between 22 and 50 meV. For single layers gaps of about 100 and 400 meV are calculated by ab initio calculations for the indirect and direct band gap, respectively. Until now, measurements have not verified the large band gaps neither for single layers nor for thin layers of $HfTe_5$. In this project, we measured band gap energies for samples with varying thicknesses and found a clear increase of gap energies for thinner samples.

We produced needle-shaped flakes of the $HfTe_5$ compound by mechanical exfoliation (see Fig. 1(b)), made electrical Cr/Au-contacts (see Fig. 1 (c) and (d)) and performed electrical measurements. The height of different samples was determined by atomic force microscope measurements (see Fig. 1(e)). Due to the strong atomic bonding and the faster growth rate in the crystallographic a-direction, we assume that the long side of the flakes is the a-axis.

In conductance-temperature measurements, we observe semiconducting behavior. From these dependencies, we extract the band gap energies E_G. For an undoped, intrinsic semiconductor, it can be assumed that the activation energy corresponds to the band gap energy E_G. So the conductance G has an exponential dependence on temperature $G \sim n \sim \exp(-E_G/(2\,k_B\,T))$ with n as the charge carrier concentration, T as the temperature and k_B as the Boltzmann constant. Afterwards, the band gap energies E_G are extracted at the linear parts in an Arrhenius plot. The resulting band gap energies with the associated sample thickness are shown in Fig. 2.

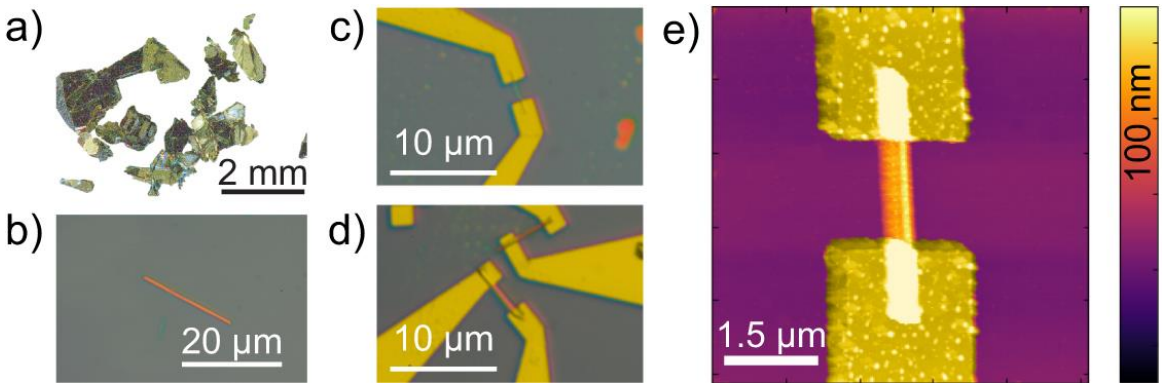

Fig.1: *(a) Optical image of synthesized bulk $HfTe_5$ crystals. (b)–(d) Optical images of different exfoliated flakes. (b) Isolated flake. (c) and (d) Cr/Au contacted flakes. (e) Atomic force microscope image of the contacted needle-shaped flake from (c).The average height is 44 nm.*

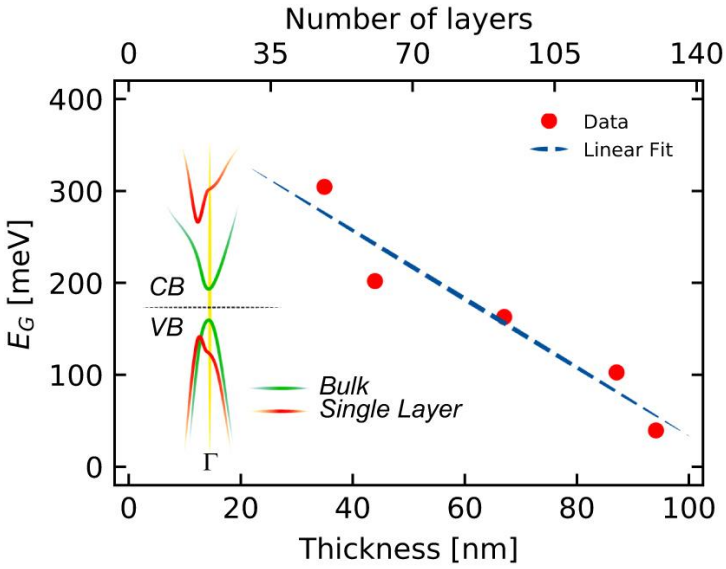

***Fig.2**: Band gap energies E_G vs. the sample thickness with a linear fit (dashed line). For decreased thickness, the band gap energy increases. Inset: schematic drawing of the band structure for bulk and a single layer $HfTe_5$ with conduction band (CB), valence band (VB) and Fermi energy E_F (dotted line) at high symmetry point Γ.*

In Fig. 2, a linear relation is seen between sample thickness and band gap energy E_G. The linear fit (dashed line) serves as a guide to the eye.

For the thinnest sample with a thickness of 35 nm we found a band gap energy of 304 meV. If we extrapolated our data to a single layer, we find a band gap of 403 meV, which is close to the predicted value of the direct band gap of a single layer. The inset in Fig. 2 shows a schematic drawing of the band structure for the bulk crystal in comparison to a single layer at the Γ-point, following.

In this project, we obtain the first experimental indication for a large band gap of about 400 meV in single layers of $HfTe_5$. The isolation of a single layer remains a special challenge, which is difficult due to poor optical visibility under the air-protecting PMMA and due to possible degradation of the material.

For further information see:

C. Belke, S. Locmelis, L. Thole, H. Schmidt, P. Behrens and R. J. Haug, *Thickness-dependent gap energies in thin layers of $HfTe_5$*, 2D Mater. **8,** 035029 (2021)