I. Physikalisches Institut (IA)
Phase-Change Materials
Prof. Dr. rer. nat. Matthias Wuttig

Topic for a Bachelor Thesis

Towards understanding the path from ordinary to exotic metals and the role of d-electrons: Characterization of NiTe-$NiTe_2$ alloys.

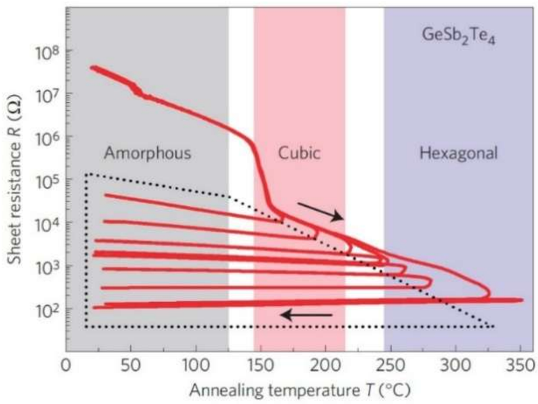

Fig 1: Sheet resistance of PCM $GeSb_2Te_4$ tracked upon different annealing temperatures. *The higher the annealing temperature was, the lower the degree of disorder and the lower the resistance. Taken from [1].*

Electrical transport properties of functional materials can be controlled and designed by understanding the bonding behavior of the compounds' electrons. The bonding character is largely governed by the outermost shell electrons (*i.e.* the valence electrons) of the material and in which way the electrons interact with each other. The degree of order of the atoms within the material has a large impact on how the electrons interact with each other. This is technically proven by phase-change materials (PCMs) which can be switched reversibly between an ordered crystalline phase and a disordered amorphous phase: In the disordered phase the (valence) p-electron orbitals between the atoms cannot align throughout the atomic network and, therefore, the electrical resistance in this phase is high (**Fig. 1**). In contrast, in the crystalline phase of PCMs the p-orbitals are aligned in such a way that electrons between atomic sites are shared and transferred to a certain degree and electrical transport is possible without large disruptions, *i.e.* the resistance is low (**Fig. 1**). In fact, with the switching between the low resistive crystalline and the high resistive amorphous phase a metal-insulator-transition (MIT) is induced.

There are many PCMs consisting of tellurides with p-bonded valence electrons like the well known PCMs Sb_2Te_3 (Antimonytelluride) or GeTe (Germaniumtelluride) and due to the high demand of PCMs for technical applications a large knowledge base about the influence of p-electrons to the bonding character has been acquired. By far less detailed knowledge about the contribution of d-electrons to the bonding character is available.

Within this thesis, a d-electron material like Nickel alloyed with different fractions of tellurium (*i.e.* $NiTe_x$, $1<x<2$) shall be investigated. While **NiTe** (**Fig. 2**) can be labelled as an ordinary metal, **$NiTe_2$** (**Fig. 2**) shows exotic metallic behavior due to its non-trivial band structure. The conduction and valence band are inverted except at certain points in the Brillouin zone where those bands are touching, which results in linearly dispersed Dirac cones at the Fermi energy. This exotic class of materials is referred to as (topological) Dirac semimetals (DSMs). It is of central interest to gain understanding about the transition from an ordinary metal like NiTe to a Dirac semimetal like $NiTe_2$ and the role of the additional Nickel d-orbitals that turn the exotic metal to an ordniary one. If the topological properties can be tuned gradually by the composition or if the transition is rather abrupt can be examined by temperature dependent electrical transport measurements.

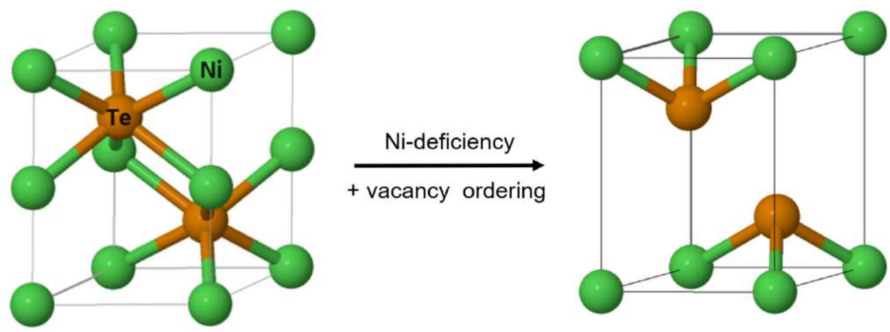

Fig 2: Unit cell of NiTe and $NiTe_2$. *When the Nickel fraction is decreased the structure gradually transitions to a layered crystal structure by incorporating a van-der-Waals layer. By that the ordinary metal turns into a Dirac semimetal (DSM), which shows exotic transport properties due to its topologically non-trivial band structure.*

Samples will be produced by plasma assisted (co-)sputter deposition and with the help of X-ray diffraction experiments the gradual change in crystal structure can be identified. Along with the change in crystal structure, the change in electrical transport behavior with special regard to topological properties at low temperatures shall be investigated.

Goals of the project: Plasma assisted sputtering and crystallization of several NiTe-$NiTe_2$ alloys, X-ray diffraction and reflection experiments for basic characterization of the produced samples, temperature dependent (2K-300K) resistivity measurements.

[1] T. Siegrist *et al.* "Disorder-induced localization in crystalline phase-change materials". Nature Materials (2011).

Christian Stenz
✉ stenz@physik.rwth-aachen.de
28 C 410 0241 / 80 27173