

Topic for a Bachelor Thesis

„Electrical transport properties of ZrTe upon structural ordering and the role of d-electrons“

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

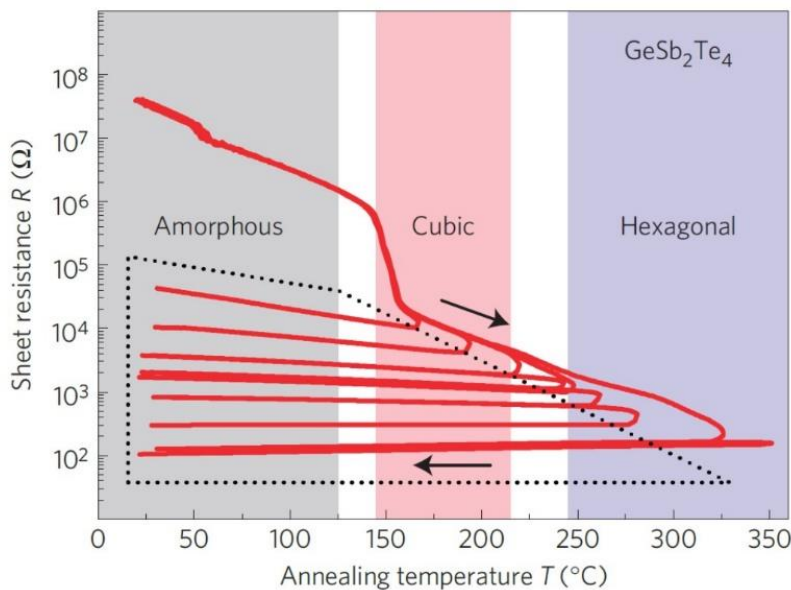


Fig 1: Sheet resistance of PCM GeSb_2Te_4 tracked upon different annealing temperatures. The higher the annealing temperature was, the lower the degree of disorder and the lower the resistance. Taken from [1].

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 zirconium alloyed with tellurium (*i.e.* ZrTe) shall be investigated upon different degrees of atomic order. Samples will be produced by sputter deposition and with the help of thermal annealing different levels of atomic order are achieved. From X-ray diffraction experiments the degree of order is determined while electrical properties like the resistance, charge carrier density or mobility are tracked via van-der-Pauw and Hall measurements.

Ultimately, a comparison of ZrTe with the prominent PCM GeTe can give new insights into the role of d-electrons for electrical transport properties, since ZrTe has two d-electrons in the valence band (originating from the Zr atoms), as compared to GeTe, which, instead, has two p-electrons in the valence band (originating from the Ge atoms).

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