

Investigation of the metavalent bonding in Phase Change Materials for electric memories

Scientific context:

Over the past two decades, Phase change Materials (PCM) have received a huge attention with various technological applications ranging from optical discs, such as commercial CD-RW or DVD-RW discs to phase-change memory (PC-RAM) [1], including more recently opportunities as all-photonic memories and flexible displays with nanopixel resolution.

Among emerging memory devices, PC-RAM are the most mature. This memory is based on a phase transition between the amorphous and crystalline states in ternary Ge-Sb-Te (GST) or pseudo binary GeTe-Sb₂Te₃ alloys making use of the large electrical and optical contrasts between the two phases, and their fast crystallization. When a voltage is applied to a device in the high-resistivity amorphous (RESET) state, it switches to the low-resistivity crystalline (SET) state. It has been shown that the role of *vacancies* and *distortions* in the metastable crystalline phase has a significant impact for the data-storage performance.

Initially, phase change materials were optimized employing empirical schemes and a trial-and-error approach. About ten years ago, however, a unique fingerprint of phase-change materials was identified [2]. All phase change materials displayed very large electronic polarizabilities in the crystalline state, which were not found in the amorphous phase. Therefore, the high values of the electronic polarizability of PCMs were attributed very recently to a new type of bonding called "*metavalent bonding*" in the crystalline state. Investigations indicate that the findings of this special bonding is a genuine mechanism in solids and not merely an intermediate (or a combination) of covalent and metallic bonding [3, 4].

Following the pioneering work of Wuttig *et al.* on the properties of the new metavalent bonding applied to binary PCMs and related materials, our goal is to extend these studies to the ternary PCMs for applications in electrical memories. A lot of attention will be paid on the role of the vacancies as well as on boundaries between the metavalent and covalent bonding.

Objective:

The project aims to develop a systematic understanding of the electrical conductivity and atomic and electronic structure in ternary tellurides as a function of stoichiometry. Relating the electrical properties to the nature of bonding and aging will provide a pathway to attractive materials for applications in PC-RAM memories.

Methodology:

-Two different groups of chemical compositions will be investigated. They correspond to different trends in chemical bonding and/or local structure. First, the study of the evolution of the material in the (GeTe)_{1-x}(GeSe)_x system starting from x=0 where metavalent bonding is expected to play a crucial role to x=1 where covalence bonding is observed. Then the investigation will focus on a second series in Ge-Sb-Te (GST) PCM by varying the composition starting from GST224 composition where no vacancy should be present [5] compared to others where the amount of vacancies varies significantly up to 28.5%.

-Amorphous films will be deposited by thermal co-evaporation technique equipped with two current induced heated sources and an electron beam evaporator. Then, different annealing treatments will be carried out in order to crystallize the amorphous films.

-Main characterizations for amorphous and/or crystalline films will include:

- * Electrical properties by employing a four-point probe and conductive atomic force microscopy (C-AFM)
- * Neutron and X-ray diffraction and EXAFS measurements (nature of the distortion)
- * Local structural order by ^{125}Te NMR (electronic structure)
- * Ab initio calculation of NMR parameters (chemical shift, Knight shift, electronic structure, ...) – WIEN2K

Collaboration:

The work will be carried out in collaboration with Matthias Wuttig (Physikalisches Institut RWTH Aachen, Germany) - PCM -, P. Blaha (TU Wien, Austria) and R. Laskowski (A*STAR, Singapore) - WIEN2K-

References:

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