

DS 40: Focus Session: Resistive Switching by Redox and Phase Change Phenomena VII (Optical properties and theory of PC materials)

Time: Thursday 11:30–13:00

Location: CHE 89

DS 40.1 Thu 11:30 CHE 89

Near-field optical investigation of Sb_2Te_3 hexagonal platelets in the mid-infrared — BENEDIKT HAUER¹, TOBIAS SALTZMANN², ULRICH SIMON², and •THOMAS TAUBNER¹ — ¹Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — ²Institute of Inorganic Chemistry (IAC), RWTH Aachen University, 52056 Aachen, Germany

Antimony telluride (Sb_2Te_3) has gained attention as a candidate for phase-change memory applications, thermoelectric devices, and as a three-dimensional topological insulator. We imaged Sb_2Te_3 hexagonal platelets grown by hydrothermal synthesis using scattering-type scanning near-field optical microscopy (s-SNOM).

In the mid-infrared spectral range between 5.5 μm and 11 μm we find a highly symmetric and very sharp pattern in both optical amplitude and phase images. This optical pattern is correlated to a growth spiral and extends over the entire platelet. We assume domains with different surface-densities of charge carriers to be the origin of the optical contrast. These domains could be caused by growth twins in the crystal lattice. On epitaxially grown Sb_2Te_3 samples we did not observe any comparable pattern.

This contribution demonstrates the unique potential of s-SNOM to visualize fundamental material properties that are hard to address with any other method.

DS 40.2 Thu 11:45 CHE 89

Large area optical tuning of mid-infrared resonant nanostructures by using low-loss phase-change materials — ANN-KATRIN MICHEL¹, PETER ZALDEN^{2,3}, •DMITRY CHIGRIN¹, AARON LINDENBERG^{2,3,4}, and THOMAS TAUBNER¹ — ¹Institute of Physics IA, RWTH Aachen University, Aachen, Germany — ²Stanford Institute of Materials and Energy Physics, SLAC, Menlo Park, USA — ³PULSE Institute, SLAC, Menlo Park, USA — ⁴Department of Materials Science and Engineering, Stanford University, Stanford, USA

Phase-change materials (PCMs) are stable in at least an amorphous and a crystalline phase. This structural contrast of PCMs is accompanied by a huge difference of the refractive index n .

So-called metallic nanoantennas are able to produce significantly enhanced and confined electromagnetic fields. By varying the fabrication parameters, such as antenna material, geometry and substrate their resonance frequency can be tuned over a wide range. If these nanoantennas are embedded in PCMs, the variation in n can be used for tuning of the resonance. To minimize any damping due to a high absorption of PCMs, we chose $\text{Ge}_3\text{Sb}_2\text{Te}_6$ as an example with a very small imaginary part ϵ_2 of the dielectric function $\epsilon(\nu)$ in the MIR [1].

Since reversible switching of the antenna resonances would allow for interesting applications e.g. in the field of plasmonics, we investigated the use of femtosecond laser pulses for reversible switching, where the huge benefit lies in the switching of several antenna arrays at the same time (total diameter ca. 270 μm^2). [1] Michel et al. Nano Lett. 13 (8), 2013.

DS 40.3 Thu 12:00 CHE 89

Understanding Stability Trends at Clean and Oxidized GeTe Surfaces — •VOLKER DERINGER¹ and RICHARD DRONSKOWSKI^{1,2} — ¹Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany — ²Jülich–Aachen Research Alliance (JARA)

Phase-change memory devices are becoming smaller and smaller, necessarily so. In turn, the surfaces of phase-change materials surely deserve increased attention: the surface–volume ratio rises dramatically on the nanoscale, and surface oxidation (detrimental to long-term switching capability) becomes important. Here, we present comprehensive DFT computations for the prototypical germanium telluride (GeTe) surfaces. We have simulated freshly cleaved and reconstructed surfaces, as well as molecular O_2 adsorption and higher oxygen coverage.

The predicted stability trends are then investigated and rationalized at the hand of chemical-bonding analysis: by partitioning the electronic structure into bonding (stabilizing) and antibonding contributions, we offer a straightforward explanation for why one type of surface termination is favorable while the other is not. This model can be directly extended to surface oxidation: more stable surfaces are rather

inert whereas others readily react with oxygen, thereby reducing unfavorable antibonding interactions at the surface. Our simulations of oxidized GeTe surfaces agree well with previous XPS measurements, and the atom-resolved and chemical-bonding techniques provide a worthwhile additional viewpoint.

DS 40.4 Thu 12:15 CHE 89

Vibrational Properties of Layered Tellurides from First-Principles Calculations — •RALF STOFFEL¹ and RICHARD DRONSKOWSKI^{1,2} — ¹Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen — ²Jülich–Aachen Research Alliance (JARA)

We present recent results of density-functional theory (DFT) based calculations of the vibrational properties of layered tellurides, such as Sb_2Te_3 and several $\text{Ge}_x\text{Sb}_y\text{Te}_z$ (GST) compounds, using the ab initio force-constant method. The latter compounds are well-known phase-change materials on the pseudo-binary tieline GeTe– Sb_2Te_3 , and they can be switched easily between amorphous and crystalline phases which significantly differ in their optical and electrical properties. Here, we discuss the thermodynamically stable hexagonal polymorphs of those GST phases. Common DFT approaches are known to fail in describing the weak, non-covalent Te–Te interactions within these layered structures. For that reason, we investigate the influence of dispersion-corrected DFT on the calculated properties. We discuss phonon properties such as band structures and densities of states as well as thermochemical data such as Gibbs free energies or heat capacities. Other derived properties will also be presented, for example Grüneisen and atomic displacement parameters. The reliability of the results is verified by comparing the theoretical data with experimental references obtained from nuclear inelastic scattering (NIS). Finally, we show how our results help to interpret experimental data, and also give a more detailed insight into the theoretical background.

DS 40.5 Thu 12:30 CHE 89

Structural phase transitions in thin films under elastic and microstructural constraints — •STEFAN WAGNER and ASTRID PUNDT — Institut für Materialphysik, Universität Göttingen

Palladium hydrogen (PdH) thin films are used as a model system to investigate the impact of elastic and microstructural constraints on structural phase transitions. Mechanical stress arises both from thin film clamping on the substrate and at coherent interfaces in phase mixtures. It changes chemical potentials, modifying phase stabilities regarding phase boundaries and enthalpies of formation. Mechanical stress is superimposed by microstructural constraints, channeling stress relaxation mechanisms such as the formation of misfit dislocations.

In this paper hydrogen absorption and hydride formation in PdH thin films with different microstructure and clamping conditions are investigated [1]. Hydrogen solubilities and phase stabilities are quantitatively related to the hydrogens' chemical potential by in-situ XRD as well as stress and electromotive force (EMF) measurement [2]. They differ for films with coherent interfaces and films where stress relaxation is possible. [1] S. Wagner, A. Pundt, Acta Mat. 59 (2011) 1862. [2] S. Wagner, M. Moser, A. Pundt et al., Int. J. Hydr. Energy 38 (2013) 13822.

DS 40.6 Thu 12:45 CHE 89

Reducing the number of domain orientations of Sb_2Te_3 on Si(111) by surface engineering — •JOS BOSCHKER¹, JAMO MOMAND², BART KOOIJ², and RAFFAELLA CALARCO¹ — ¹Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — ²Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

The epitaxy of interfacial phase change memory [1] requires a detailed understanding of the stacking of van der Waals solids (Sb_2Te_3) with 3-dimensional solids (GeTe). Here we use to growth of Sb_2Te_3 on Si(111) as a model system for studying this kind of epitaxy. We show that Sb_2Te_3 grown on Si(111)-(7 \times 7) exhibits ten different domain orientations, even though only one is expected based on the symmetries of the two materials. We show that the in-plane rotations are due to the formation of a coincidence lattice between Sb_2Te_3 and the dangling

bonds on the Si(111)-(7x7) surface. Furthermore, we demonstrate that the number of domain orientations can be reduced to two when Sb₂Te₃ is grown on Si(111)-($\sqrt{3}\times\sqrt{3}$)R30°-Sb or Si(111)-(1x1)-H. Finally, in-plane rotations of ultrathin Sb₂Te₃ layers on Si(111)-(7x7) and Si(111)-($\sqrt{3}\times\sqrt{3}$)R30°-Sb are determined using angular resolved RHEED. This detailed understanding of the epitaxy of Sb₂Te₃ on Si(111) is impor-

tant for the growth of Sb₂Te₃/GeTe superlattices and thus for the optimization of interfacial phase change memory.

[1] R. E. Simpson, P. Fons, A. V. Kolobov, T. Fukaya, M. Krbal, T. Yagi, and J. Tominaga, Interfacial phase-change memory, *Nat. Nanotechnol.*, vol. 6, pp. 501-5, Aug. 2011.