Bulk ESCA and Valence Band measurements of Ge-Sb-Te based Optical Memory Alloys

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Phase-change alloys based upon chalcogenide compounds are now in wide use as re-writable optical media. Ge-Sb-Te compounds, specifically those lying along the ZnS—SiO_2 pseudo-binary tie-line are known to exhibit nanosecond scale transitions between the crystalline and amorphous phases and are now in widespread commercial use. Despite their wide use and over thirty-five year history, the properties of the utilized phase transition are only now becoming understood. We recently proposed a structural model (Nature Materials 3(10), 703 (2005)) that describes the local ordering changes occurring in the amorphous-crystalline phase transition based upon our measurements at Spring-8 on the Ge-Sb-Te alloy $Ge_2Sb_2Te_5$. We believe our model is general and with minor modifications can also describe the local structuralchanges occurring in other Ge-Sb-Te alloys.

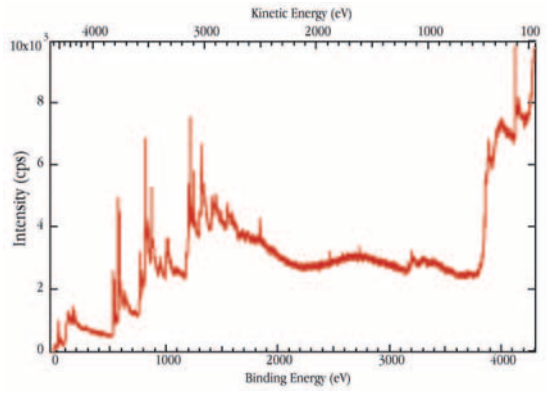
As a first step, it is important to investigate the electronic structure of $Ge_2Sb_2Te_5$ in particular and optical memory alloys in general. Using the structures recently determined by our group, we intend to use ab-initio calculations to determine the corresponding electronic structure of these materials. The importance of doing such calculations is underscored by the need to understand both the origin of *kinetic* barriers to the phase transition process and hence the speed with with optical memory alloys can be switched, as well as to confirm our strong belief that *electronic excitation* associated with phasetransition inducing laser light also plays an important role in phase transition reversibility. Both of these areas can only be addressed by a more complete knowledge of both crystallographic and electronic structure. The experimental valence band density of states and chemical state data to be determined by these experiments will provide critical feedback for the development of such electronic structural models. In particular, we wish to explore further the origin of kinetic barriers for the amorphous to crystalline phase transition, the possibility of a ferroelectric transitions and the influence of impurities/alloys on optical memory performance to a name a few topics of interest.

We have measured both XPS and valence spectra for $Ge_2Sb_2Te_5$optical memory alloys in both the laser-induced amorphous and metastable crystalline states. The sample structure consisted of Al-Cr

(100)/ ZnS-SiO2(30)/ Ge2Sb2Te5(20)/ ZnS-SiO2(130)/ polycarbonate substrate (distances are in nm). Samples were grown by sputter deposition. The as-grown sample was then mounted in a Pulstec ddu unit. Two different annuli of approximately 10 mm width were then laser-amorphized and laser-crystallized, respectively. This assured that the both the amorphized and crystallized samples were of the same composition. The samples were delaminated in a nitrogen glove box at BL15XU to expose the top surface of the $Ge_2Sb_2Te_5$ recording layer and were transported to the beamline load 2004B0411-Nsa-np-Na

lock chamber without atmospheric exposure. Samples were affixed to the sample blocks using conductive carbon tape. The samples were excited just below the Sb L2 edge to avoid peak interference effects using a 4345 eV helically polarized xray beam with a resolution in energy of 1:10000. By using this excitation energy, it proved possible to sample a reasonable subspace of ESCA and AES peaks allowing the use of Auger parameter analysis. The x-ray beam spot size was approximately 5 by 10 millimeters on the sample. No polarization effects are expected in this experiment as the samples had random (poly) crystalline orientations in the lasercrystalline phase. It should also be noted here that the irradiation of the substrate by the x-ray beam was found to discolor the polycarbonate layer implying the occurrence of x-ray induced depolymerization or x-ray beam induced heating. This distortion in the substrate may be of concern to future experimenters and thus is reported here.

Figure 1 shows a typical survey spectra observed from the as-loaded sample. No oxygen peak was



Typical survey data from a Ge2Sb2Te5 laser-crystallized film

observed indicating that the decapping procedure in a Nitrogen ambient was effective. Some slight charging effects were observed for the amorphized sample due to its low conductivity, but these were easily compensated for using an electron flood gun. Valence-band density of states were also taken.