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Composition of complex amorphous insulators from ab initio calculations and X-ray photoelectron spectra

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Abstract – We report density functional theory calculations (DFT) of core level shifts (CLS) in amorphous $CdTeO_x$ (x=0.2,1,2, and 3). Using the CLS, we compute the X-ray photoelectron spectra and develop a method to determine the composition by comparison of the theoretical and experimental spectra. We conclude that the correlation between the area ratios of tellurium peaks in the CLS spectrum and the oxygen concentration does not obey simple rules. Hence, computer simulations are needed in order to obtain concentrations correctly in experimental samples.

In this study we perform DFT calculations for the composities reported in [1] by using an structural model for amorphous CdTe oxides studied in [2]. The area under a XPS peak is proportional to the number of species in a particular environment. This makes it difficult to deduce atomic ratios and chemical compositions directly from XPS since the environments of atoms also depend on the structure. In an experiment, the chemical composition is often very difficult to control in detail and may, for example, depend on the pressure of a gas during the manufacturing process. It is particulary difficult to deduce chemical compositions in amorphous materials since the structures are unknown on an atomic level. We obtain the oxigen content by comparing the experimental and calculated XPS spectra. We illustrate this for amorphous $CdTeO_x$, where we deduce the correct oxigen concentration as function of NH_3 partial pressure in an Ar-NH_3 sputtering plasma as reported in [1].

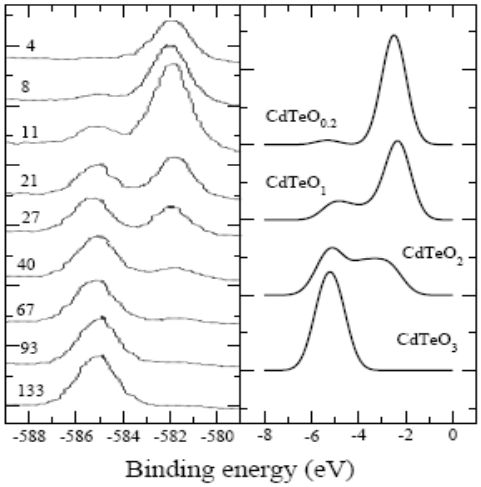

Figure 1: A comparison between the experimental and theoretical spectra. On the left side for different NH_3 partial pressure and on the right side for several oxygen contents.

References

[1] P. Bartolo-Pérez, R. Castro-Rodríguez. F. Caballero-Briones, W. Cauich, J. L. Peña and M. H. Farías, Surface and Coatings Technology 155 16-20 (2002).
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