XPS study of oxygen non-stoichiometry in some II-VI Oxides

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Although HAXPES focusses on photoelectron spectroscopy (PES) with synchrotron based hard x-rays (HAX) "up to and beyond 10 keV", a laboratory based x-ray photoelectron spectroscopy (XPS) study using 1.2536 keV x-ray of differently fired Magnesium Oxide, Zinc Oxide and Cadmium Oxide II-VI semiconductors seems to reveal interesting information for follow up experiments. It shows significant changes in room temperature stoichiometry and electronic structure resulting from the heat treatments. Doping of a suitable 3rd element in a II-VI semiconductor like zinc oxide to generate p- or n-type carriers and tailor the band gaps is a very competitive field of research in view of their potential use as electronic material and as TCO in solar cells. However, possible non-stoichiometry in the II-VI host, as observed [1] in differently heat treated cadmium oxide, causes doping without adding a 3rd element. Since this self-doping due to non-stoichiometry must be fully known before taking up any impurity-doping project, it has been investigated for above oxides by XPS and associated techniques. Fired cadmium oxide also showed marked a reduction [1] in electrical conductivity.

XPS data were obtained using non-monochromatic MgK_α ($h\nu$ = 1253.6 eV) excitation source in ESCA-2000 Multilab apparatus (VG Microtech) with a residual gas pressure in the range of 10^{-10} Torr. All spectra were taken at room temperature and were separated by a concentric hemispherical analyzer (CHA) under 0° take-off angle together with pass energy of 50 eV and an instrumental resolution of 0.6 eV. The binding energies have been corrected for sample charging effect with reference to the C 1s line at 284.5 eV for the surface of the oxide.

Cd and O lines seem to indicate mostly O-loss for firing at different temperatures up to 800° C. Cd atomic %, as found from this XPS for the as-supplied Aldrich cadmium oxide, is 52.6%, and increases to 61.9% after 36 H of 800° C firing. On the other hand, XPS shows Zn / O = 2.146 for ZnO-400 or the 400° C fired zinc oxide sample reducing to Zn / O = 1.426 for ZnO-700 or the 700° C fired sample or relative gain in O-concentration. XPS on differently fired magnesium oxide shows Mg/O = 0.6494 for MgO_200 reducing to Mg/O = 0.4082 for MgO_800 i.e. relative gain in O-concentration due to heat treatment. These finding have been compared with results from other analytical techniques.

[1] Udayan De, K.C. Verma, P. Karmakar, A. Sarkar, Soma Dey and SikhaVerma, Nuclear Instru. & Methods in Phys. Res. B 212 (2003) 505; [2] Udayan De and K.C. Verma, Proc. of the "15th National Symp. on Thermal Analysis", Jaipur (India), 6-8 Feb. 2006, c/o Indian Thermal Anlysis Society.