Energy band mapping in ETA cells

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ETA cells (Extremely Thin Absorber solar cells) are solar cells where the light absorber is a semiconductor deposited as a thin layer on a porous, high surface area charge conductor (usually an electron conductor) and a charge conductor of the opposite type is infiltrated into the porous structure. Common examples of ETA cells use TiO_2 or ZnO as electron conducting porous substrate, light absorbing metal sulphides or selenides as absorber and CuSCN as hole conductor.

Many studies on ETA cells are largely empirical in nature. More recently, kinetics of charge transfer processes are being studied. However, energy band mapping and alignments, a critically important issue, have not been often studied in ETA cells. Where such band diagrams have been given, they most often are taken from known (or assumed) energy band parameters of the individual components without taking into account possible interactions between the different components.

Here we describe mapping of such energy band structures for some ETA cells based on (mainly) XPS, UPS and Kelvin probe measurements. We first extract the surface and subsurface work function variations across the heterostructure and, similarly, the top of valence band energies. Furthermore, using a recent method, chemically resolved electrical measurements (CREM)¹, we exploit a common problem associated with electron spectroscopy, the spectral distortions under differential charging, to gain detailed understanding of the major charge-trapping characteristics and the evolving internal fields. Irreversible changes associated with the exposure of the sample to the XPS x-ray source and to the electron flood gun were studied and eliminated. We also inspected instabilities appearing under vacuum conditions and under inert or ambient atmosphere.

The present method is particularly effective in studies of granular heterostructures. We have found that the inhomogeneous morphology of ETA cells often allows detection of layers 'buried' much deeper than the nominal few nm limit typical to photoelectron spectroscopy. This allows us to follow the photoelectron peaks of previously-deposited layers as new layers are deposited.

Regarding possible differences in band structures between the UHV of the spectrometer and actual cells, the main tool we have to check this is to compare work functions measured in the spectrometer and those measured by Kelvin probe in a controlled atmosphere.

Examples are presented of energy band structures of ETA cells and part cells that provide not only the overall band structure of the cells (or the partial cells) but also illustrate how these techniques can provide information on electric fields in the cell, diffusion of species from one part of the cell to another and shed light on the mechanism of the important K(Li)SCN treatment of these cells.

References

1. H.Cohen, "Chemically Resolved Electrical Measurements using X-ray Photoelectron Spectroscopy", *Applied Physics Letters* **85**, 1271-3 (2004).