AIP | Conference Proceedings

Electronic and structural properties of the surfaces and interfaces of indium oxide

Aron Walsh

Citation: AIP Conf. Proc. **1399**, 189 (2011); doi: 10.1063/1.3666319
View online: http://dx.doi.org/10.1063/1.3666319
View Table of Contents: http://proceedings.aip.org/dbt/dbt.jsp?KEY=APCPCS&Volume=1399&Issue=1
Published by the American Institute of Physics.

Related Articles

Efficient polymer solar cell employing an oxidized Ni capped Al:ZnO anode without the need of additional hole-transporting-layer
Appl. Phys. Lett. 100, 013310 (2012)

Efficient polymer solar cell employing an oxidized Ni capped Al:ZnO anode without the need of additional hole-transporting-layer
APL: Org. Electron. Photonics 5, 10 (2012)

Impact of unbalanced charge transport on the efficiency of normal and inverted solar cells
Appl. Phys. Lett. 100, 013306 (2012)

Impact of unbalanced charge transport on the efficiency of normal and inverted solar cells
APL: Org. Electron. Photonics 5, 6 (2012)

Can morphology tailoring improve the open circuit voltage of organic solar cells?
Appl. Phys. Lett. 100, 013307 (2012)

Additional information on AIP Conf. Proc.

Journal Homepage: http://proceedings.aip.org/
Journal Information: http://proceedings.aip.org/about/about_the_proceedings
Top downloads: http://proceedings.aip.org/dbt/most_downloaded.jsp?KEY=APCPCS
Information for Authors: http://proceedings.aip.org/authors/information_for_authors

ADVERTISEMENT

AIPAdvances

Submit Now

Explore AIP's new open-access journal

- Article-level metrics now available
- Join the conversation! Rate & comment on articles

Downloaded 19 Jan 2012 to 138.38.25.124. Redistribution subject to AIP license or copyright; see http://proceedings.aip.org/about/rights_permissions

Electronic and structural properties of the surfaces and interfaces of indium oxide

Aron Walsh

University College London, Department of Chemistry, Materials Chemistry, Third Floor, Kathleen Lonsdale Building, Gower Street, London WC1E 6BT, United Kingdom; Laboratory for Computational Physical Sciences and Surface Physics Laboratory, Fudan University, Shanghai 200433, China

Abstract. Indium sesquioxide is a transparent conducting oxide material widely used in solar cell and solid-state lighting devices. Following our recent successes in modeling the electronic and defect properties of In_2O_3, we report an investigation of the surface physics of this material. In the ground-state bixbyite phase, the surface energies follow the order $(100) > (110) > (111)$, with the charge neutral (111) termination being the lowest energy cleavage plane; the same ordering preferences have been established for materials adopting the parent fluorite (AB_2) structure. Our first-principles predictions, based on density functional theory, are confirmed through collaboration with the group of Russell Egdell at Oxford University, who grew epitaxial In_2O_3 single crystals on lattice matched $(100), (110)$ and (111) Y-stabilized zirconia substrates, and observed that (111) facets spontaneously form on other low index terminations. Furthermore, we have performed work function analysis of the low index In_2O_3 surfaces using a hybrid density functional, which is found to be in very good agreement with recent experiments.

Keywords: Metal Oxides, ITO, Density Functional Theory, Defects, Solar Cells
PACS: 77.84.Bw, 68.47.Gh, 71.15.Dx, 31.15.E-, 81.15.Hi

The combination of optical transparency in the visible range with low levels of electrical resistivity define transparent conducting metal oxides (TCOs). Indium sesquioxide is a leading TCO material, which arises due to its high electron affinity and low electron effective mass, making it both intrinsically *n*-type and highly susceptible to extrinsic electron doping, *e.g.* Sn-doped In_2O_3 (ITO). While its fundamental electronic band gap has recently been revised to *ca.* 2.9 eV[1], transparency is maintained through a combination of dipole forbidden band edge optical transitions, which also manifest themselves in bulk and amorphous ternary indium oxides, including the solid solution of In_2O_3 and ZnO (IZO)[2, 3, 4].

The ground-state crystal structure of In_2O_3 is bixbyite ($Ia\bar{3}$), although a number of denser high pressure phases exist[5]. Bixbyite can be viewed as a $2 \times 2 \times 2$ expansion of the fcc fluorite structure, with $\frac{1}{4}$ of the anion sites vacant. The resulting cubic lattice constant is 10.117 Å, and there are 80 atoms in the unit cell.

Here we present a summary of new insights into the surface physics of In_2O_3, which will also be relevant to other sesquioxide materials, as well as the In_2O_3 interfaces widespread in contemporary optoelectronic devices; the detailed results will be presented elsewhere.

Calculations were performed using density functional theory[6, 7] as implemented in the VASP code[8], with the PBE exchange-correlation functional[9]. The surfaces were modeled as 2D slabs with a 20 vacuum layer separating periodic images. For the polar (100) surface, the dipole was quenched through microfaceting (*e.g.* see related work on the (111) surface of MgO[10]). Estimations of the surface potentials and band gaps were obtained using a screened exact-exchange hybrid density functional (HSE06)[11].

The ideal (100), (110) and (111) terminations of the fluorite structure are shown in Figure 1, along with the relaxed surface energies, ionization potentials and surface band gaps of bixbyite In_2O_3, which allow us to make the following observations:

- The (111) termination is thermodynamically favored, with the microfaceted (100) surface highest in energy.
- The calculated surface energies agree with the observed morphologies of single crystal thin films grown on Y-stabilised ZrO_2[12].
- The ionization potentials vary between 7.2 and 7.9 eV, in good agreement with recent measurements (*ca.* 7.1 eV for polycrystalline samples)[13].
- While an insulating band gap is maintained, surface states reduces the band gap by $0.4 - 1.1$ eV; the origins of this reduction will be explored in future work.

In_2O_3 is a complex oxide material; however, through the combination of theory and experiment, we are beginning to have a better grasp of its underlying physicochemical properties, which will help both in our understanding of its role in technological devices, and the ra-

Physics of Semiconductors
AIP Conf. Proc. 1399, 189-190 (2011); doi: 10.1063/1.3666319

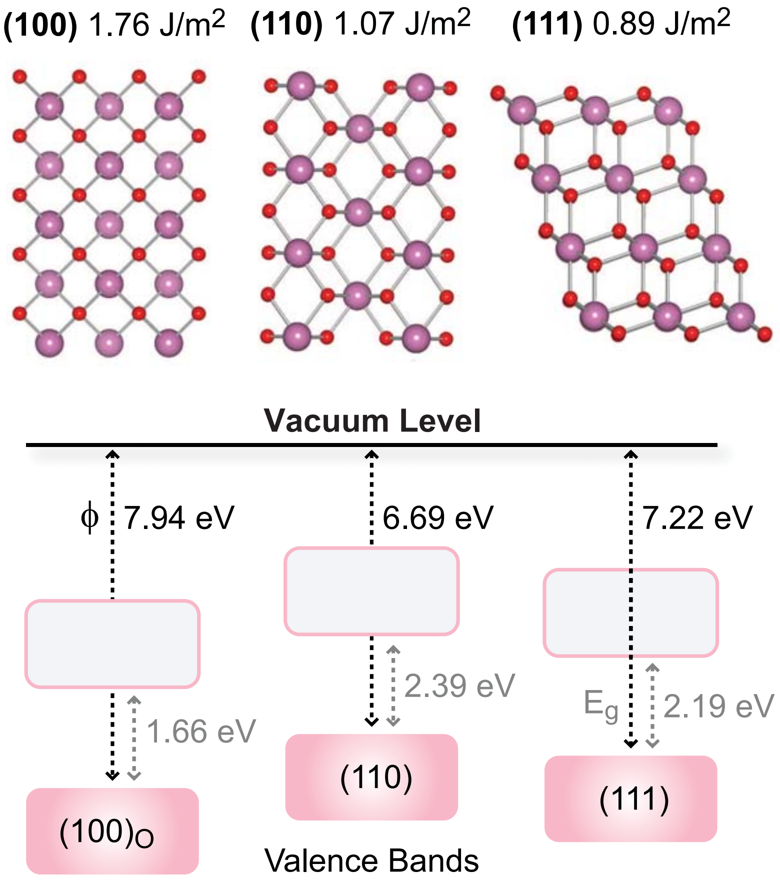

FIGURE 1. Schematic of the ideal fluorite surface terminations (upper panel), which are directly related to those of bixbyite In_2O_3, along with the calculated surface energies and potentials of In_2O_3 (lower panel).

tional design of alternative TCO materials.

ACKNOWLEDGMENTS

I acknowledge stimulating discussions with D. Demathieu, H. Zhang, R. G. Egdell and C. R. A Catlow. The work was funded through a Marie-Curie Fellowship from the European Union, and an International Young Scientist Fellowship from the NSF of China (Grant 10950110324). The work utilized HECToR through membership of the UK's HPC Materials Chemistry Consortium, which is funded by EPSRC (Grant EP/F067496).

REFERENCES

1. A. Walsh *et al.*, *Phys. Rev. Lett.* **100**, 167402 (2008).
2. A. Walsh, J. L. F. Da Silva, and S.-H. Wei, *Chem. Mater.* **21**, 5119 (2009).
3. A. Walsh, J. L. F. Da Silva, Y. Yan, M. M. Al-Jassim, and S.-H. Wei, *Phys. Rev. B* **7**, 073105 (2009).
4. D. H. O'Neil, A. Walsh, R. M. J. Jacobs, V. L. Kuznetsov, R. G. Egdell, and P. P. Edwards, *Phys. Rev. B* **81**, 085110 (2010).
5. A. Walsh, C. R. A. Catlow, A. A. Sokol, and S. M. Woodley, *Chem. Mater.* **21**, 4962 (2009).
6. W. Kohn, and L. J. Sham, *Phys. Rev.* **140**, A1133 (1965).
7. P. Hohenberg, and W. Kohn, *Phys. Rev.* **136**, B864 (1964).
8. G. Kresse, and J. Furthmüller, *Phys. Rev. B* **54**, 11169 (1996).
9. J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).
10. D. O. Scanlon, A. Walsh, B. J. Morgan, M. Nolan, J. Fearon, and G. W. Watson, *J. Phys. Chem. C* **111**, 7971 (2007).
11. A. V. Krukau, O. A. Vydrov, A. F. Izmaylov, and G. E. Scuseria, *J. Chem. Phys.* **125**, 224106 (2006).
12. A. Bourlange, D. J. Payne, R. G. Egdell, J. S. Foord, P. P. Edwards, M. O. Jones, A. Schertel, P. J. Dobson, and J. L. Hutchison, *Appl. Phys. Lett.* **92**, 092117 (2008).
13. A. Klein, C. Korber, A. Wachau, F. Sauberlich, Y. Gassenbauer, R. Schafranek, S. Harvey, and T. O. Mason, *Thin Solid Films* **518**, 1197 (2009).