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Simulating the role of novel transparent conductive oxides for heterojunction solar cells

Geedhika K. Poduval[1], Bram Hoex[1]

[1]*University of New South Wales, Sydney, Australia*
E-mail: g.poduval@student.unsw.edu.au

Heterojunction (HET) silicon solar cells consist of crystalline silicon (c-Si) wafers as the absorber layer and intrinsic and doped amorphous (a-Si) or microcrystalline (mc-Si) silicon thin layers as passivating contacts. These layers are electrically and optically coupled with the metal electrodes on top using a transparent conductive oxide (TCO). As the doping efficiency of a-Si is relatively low, TCOs are required to enhance the lateral carrier transport to the contacts while maintaining a high transmission of visible and near-infrared light to the c-Si absorber.

Indium tin oxide (ITO) is the most widely used TCO due to its excellent electrical properties. Nonetheless, the high and increasing cost of indium and high carrier density leading to significant optical absorption due to free carrier absorption motivates the development of new TCO materials with even higher carrier mobility or significantly lower costs. Over the recent years, various other materials have been investigated such as doped In_2O_3, doped ZnO, SnO, doped Cu_2O, TiO_2, CdO, etc. However, most of these materials are studied for applications in optoelectronic devices such as LED displays and have not been investigated for application in HET solar cells. While selecting a new TCO for HET solar cells, the following aspects should be studied:

- Large band gap to minimise absorption due to band-to-band transitions in the visible range which in turn reduce cell current.
- Band line up and optimal charge transport at the TCO/a-Si:H interface
- High mobility with low carrier concentration to limit free carrier absorption.

The experimental constraints in evaluating all these effects for a variety of TCO is the motivation for the simulation approach taken in this work. Among the various solar cell simulators available, AFORS-HET (**A**utomat **for s**imulation of **het**erostructures) is tailored to handle homo and heterojunctions solar cells. This open source software can solve the semiconductor equation for any system at thermodynamic equilibrium, at steady state or transient conditions and with an external applied voltage and/or illumination that is constant, pulsed or sinusoidal. Additionally, it can calculate internal cell characteristics, such as band diagrams, local generation/recombination rates, local cell currents, carrier densities, phase shifts. Furthermore, characterisation methods such as current-voltage, internal external quantum efficiency, intensity and voltage dependent surface photovoltage, photo and electroluminescence, impedance spectroscopy, electrical detected magnetic resonance, capacitance/conductance decay among others, can be simulated.

In this work, the influence of various TCOs on the overall HET solar cell performance is simulated using AFORS-HET. The cell layout being investigated is Ag/TCO/a-Si:H/C-Si/a-Si:H/TCO/Ag with doped ZnO as the TCO. By modulating the work function, band gap and carrier effective mass of the TCO layers, we will engineer the electronic band to enhance carrier selectivity and mobility. Al, Si doping in ZnO has experimentally shown high transmittance and conductance along with high electron selectivity which will be verified computationally. The influence of the material properties on the overall cell performance with respect to that of ITO as TCO will also be addressed. The success of this work would pave the path for novel carrier selective TCOs for heterojunction solar cells.