Evaluation of TiO$_2$ as Carrier Selective Contact for High Efficiency Photovoltaic Applications

Alexander Rosner
Electrical Engineering, University of Notre Dame

NNIN REU Site: ASU NanoFab, Arizona State University, Tempe, AZ
NNIN REU Principal Investigator: Dr. Mariana Bertoni, Electrical Engineering, Arizona State University
NNIN REU Mentor: Dr. Laura Ding, Electrical Engineering, Arizona State University
Contact: arosner@nd.edu, mariana.bertoni@asu.edu, laura.ding@asu.edu

Abstract:

Herein we evaluate titanium dioxide (TiO$_2$) as a carrier selective contact for silicon solar cells. Additionally, we investigate aluminum oxide (Al$_2$O$_3$) as a dedicated passivation layer that could be combined with TiO$_2$ for improved performance. Using a photoconductance lifetime tester, we found that TiO$_2$ presents a poor passivation of the silicon surface and that the best minority carrier lifetime was achieved on an 8 nm thick Al$_2$O$_3$ layer annealed in forming gas. We then created heterojunction with intrinsic thin (HIT) solar cells using TiO$_2$ as the electron carrier-selective contact, and found low open-circuit voltages and efficiency consistent with the poor surface passivation.

Introduction:

The most efficient silicon solar cell today uses amorphous silicon (a-Si) to passivate the surface and selectively collect carriers from the c-Si. However, a-Si absorbs some of the light that the c-Si could turn into carriers. We investigated TiO$_2$ as a replacement candidate since, with a band gap of 3.2 eV, it is transparent to visible light and its bandstructure theoretically should line up with c-Si's, making it a good electron-selective contact [1]. However, TiO$_2$'s ability to prevent surface recombination of minority carriers is variable and our project’s aim was to quantify it.

Experimental Procedure:

We prepared TiO$_2$ and Al$_2$O$_3$ films using thermal atomic layer deposition (ALD) on n-type Czochralski c-Si wafers after removing the native oxide. We varied the deposition temperature and film thickness to investigate the relationship between films' properties and passivation capability. Next, we annealed the wafers to activate the passivation and varied the annealing temperature, duration and atmosphere (air or forming gas). The films were deposited on both sides of the wafer for lifetime measurement, while only on the back side of the cells.

We evaluated surface passivation of c-Si by quasi-steady-state photoconductance decay measurements to extract the minority carrier lifetime, at a minority carrier density (MCD) of $1 \times 10^{15}$ cm$^{-3}$.

We report effective lifetimes ($\tau_{eff}$), which account for bulk and surface lifetimes. Solar cell performances were characterized by current-voltage and by external quantum efficiency (EQE) measurements.

Results and Conclusions:

The effective lifetimes of the different thicknesses of TiO$_2$ prepared at different temperatures are presented in Figure 1, for the as-deposited state and after annealing. The highest lifetimes originate from the thinnest coatings, and annealing has only a minor effect for 3 min, while a drop in lifetime was observed for 30 min. The detrimental impact of thicker layers and longer annealing is possibly related to stress-induced phase transformation leading to more defects in the films and a higher recombination rate [2]. The deposition temperature seems to have no effect on the passivation quality. Using TiO$_2$, we could only achieve a surface recombination velocity of 70 cm.s$^{-1}$, whereas a-Si can produce > 1 cm.s$^{-1}$ (15 cm.s$^{-1}$ in our case).

We prepared cells with the best TiO$_2$ films—8 nm (230°C), 5 nm (180°C), 6 nm (130°C)—as the electron-selective contact. Figure 2 shows the EQE of the best cell compared to two reference cells, a standard HIT and HIT with Al back. At higher wavelengths, the current generated by the cell with TiO$_2$ is lower than that of the references mainly because of a difference in back side light reflection.

Figure 3 shows a table of the solar cells' performance. The TiO$_2$ thickness-dependence was only observed in the fill factor (FF), due to the high resistivity of TiO$_2$ (typically $\sim 10^5$ $\Omega$.cm), with the thinnest TiO$_2$ layer resulting in a FF as high as the reference cells. All open-circuit voltage ($V_{oc}$), short circuit current density ($J_{sc}$) and efficiencies were lower than for the reference cells. The $V_{oc}$ of the best TiO$_2$ cell was 564 mV, which is comparable to the implied $V_{oc}$ value (given by the lifetime tester as the highest $V_{oc}$ attainable by the cell if passivation is the only limiting
factor) of 580 mV. This demonstrates that the passivation and not the carrier selectivity is the most significant factor in poor cell performance. Therefore, Al₂O₃ was investigated as an alternative passivation coating.

In Figure 4, we show the lifetime of Si wafers with different thicknesses of ALD Al₂O₃ against different annealing conditions. We found that 8 nm thick films lead to the best lifetime > 1 ms after a 15 min 425°C anneal in forming gas. Although annealing in air revealed that thicker layers (15 and 3 nm) result in better passivation as they contain more hydrogen to passivate the dangling silicon bonds, this advantage decreases when hydrogen can be provided by annealing in forming gas [3]. Moreover, thicker layers may suffer from increased stress, explaining why the 8 nm thick film gave the best passivation.

In summary, we found that the poor passivation ability of TiO₂ on silicon for a wide range of depositions and post-deposition treatment conditions resulted in underperforming solar cells, however the passivation ability of Al₂O₃ seems to be comparable to α-Si, presenting a potential path for high efficiency devices.

**Future Work:**
We would like to combine Al₂O₃ and TiO₂ layers, and implement them at the sun-facing side instead of backside to improve passivation and benefit from higher transparency than the α-Si layers. Changing the deposition method or trying different post-deposition treatments such as light-soaking could improve the passivation ability of TiO₂.

**Acknowledgements:**
I would like to thank my PI, Dr. Mariana Bertoni, my mentor, Dr. Laura Ding, and Simone Bernardini for all of their help and guidance. I also want to acknowledge the National Nanotechnology Infrastructure Network Research Experience for Undergraduates Program and the National Science Foundation for making this research possible under Grant No. ECCS-0335765.

**References:**