Exploiting Fixed Charge to Control Schottky Barrier Height in Si|AlO\textsubscript{x}|MoO\textsubscript{x} – based Tunnel Diodes

Ben M. Garland, Benjamin E. Davis, Nicholas C. Strandwitz
Materials Science and Engineering, Lehigh University

Introduction
Carrier selective contacts have become one of the leading advancements in photovoltaics with the most efficient structures exceeding 26% conversion efficiency [1]. Carrier selectivity increases the efficiency and cost effectiveness of solar cells by reducing recombination at metal contacts and avoiding highly doped emitter layers. Popular selective contact materials are often transition metal oxides (TMOs) [2,3]. In contrast to previous articles, recent studies have indicated that the interface of p-type silicon and molybdenum oxide (MoO\textsubscript{x}) exhibits a significant Schottky barrier ($\Phi_{bh}$) that decreases the efficiency of hole-selective contacts by impeding majority carrier hole collection. To alleviate this issue, the current work utilizes atomic layer deposited (ALD) alumina (Al\textsubscript{2}O\textsubscript{3}) between Si wafer and MoO\textsubscript{x} with the expectation to generate a negative interface fixed charge ($N_f$) after annealing, decreasing band bending and increasing hole selectivity [1,4]. ALD alumina also provides passivation to decrease interface trap state density ($D_{it}$) with diffusion of precursor hydrogen during annealing [5-7].

Sample Preparation

- MOSCAP for $N_f$ quantification:
  - MOSCAP for $\Phi_{bh}$ quantification:
  - Tunnel diodes for $\Phi_{bh}$ quantification:
  - Si surface preparation:
    - SC-1, SC-2 (RCA-terminated)

Atomic layer deposition (ALD):
- Al\textsubscript{2}O\textsubscript{3}: Trimethylaluminum (TMA) (TMAl) and H\textsubscript{2}O (at 80-300°C)
- MoO\textsubscript{x}: Bis(ethyl-ylidimino)bis(dimethylamido)Mo and O\textsubscript{2} at 200°C

MOSCAP electrical analysis

$N_f$ from capacitance-voltage (C – V)

- As-deposited samples have less negative $N_f$ compared to annealed samples, with lower deposition temperature annealed samples having largest $N_f$.
- $\Phi_{bh}$-Terman method (C – V)

Tunnel diode electrical analysis

Current-density-voltage (J – V) diode rectification

- n- and p-type Si tunnel diodes exhibited opposite trends in current density with alumina processing, aside from n-type at high reverse bias.
- Possibly coincides with $N_f$ changes from C – V measurements, though Rs was found to be high.

Tunnel diode $\Phi_{bh}$ summary

- $\Phi_{bh}$ is dependent on a negative $N_f$ and is shown to be controlled with processing
- n-type Si barrier height can be increased
- Effect in p-type Si remains inconclusive
- May be too small to measure by Mott-Schottky method.

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References