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Investigation of atomic-layer-deposited TiO_x as selective electron and hole contacts to crystalline silicon

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Abstract

The applicability of atomic-layer-deposited titanium oxide (TiOx) thin films for the formation of carrier selective contacts to crystalline silicon (c-Si) is investigated. While relatively good electron selectivity was presented recently by other groups, we show that carrier selectivity can be engineered from electron to hole selective depending on the deposition conditions, post deposition annealing and the contact material covering the TiOx layer. For both the electron and hole contacts, an open-circuit voltage (Voc) of ~ >650 mV is obtained. The fact that the Voc is correlated with the (asymmetric) induced c-Si band bending suggests that carrier selectivity is mainly governed by the effective work function and/or the fixed charge rather than by the asymmetric band offsets at the Si/TiOx interface, which provides important insight into the basic function of metal-oxide-based contact systems.

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Keywords: Titanium oxide; atomic layer deposition; crystalline silicon; solar cell; carrier selective contact

1. Introduction

Carrier selective contact that extracts one type of carrier (electron or hole) out of the light-absorbing material is a subject of current interest for photovoltaic application [1]. In particular, novel carrier selective contacts for crystalline silicon (c-Si) can be used to replace the conventional p-n homojunction and hydrogenated amorphous

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silicon (a-Si:H)/c-Si heterojunction schemes for achieving high efficiency without complex device processing. While various high-work-function transition-metal-oxides such as MoO_x, WO_x, and V_2O_x have been demonstrated as hole selective contacts for c-Si solar cells [2-4], efficient electron selective contact has been lacking. Recently, TiO_x (or TiO_2) thin-layers deposited by atomic layer deposition (ALD) [5] or chemical vapor deposition [6,7] have been reported to act as electron selective contacts to crystalline silicon solar cells. Yang *et al*. demonstrated a 21.6% efficient solar cell by applying a thermal-ALD TiO_x to full-area rear electron contact for N-type monocrystalline silicon base [5]. The origin of the electron selectivity of TiO_x has been ascribed to the asymmetric current flow at the Si/TiO_x interface where the low conduction band offset allows the electron flow while the high valence band offset hinders the hole flow [5-7]. Meanwhile, it is suggested that ALD-TiO_x contain negative fixed charge [8,9], which might be detrimental in aiming for an ideal electron selective contact. In this work, we have investigated the carrier selectivity of TiO_x prepared by ALD with different oxidation processes using oxygen plasma and thermal reaction with H_2O vapor. Our results show that the carrier selectivity of TiO_x is widely tunable from electron-selective (V_{oc}~680 mV) to hole-selective (V_{oc}~650 mV) by the ALD process, post-deposition treatments and contact material that covers TiO_x layer.

2. Experiment

We fabricated solar cell precursors as shown in Fig. 1. Si wafers (N-type float zone silicon, 1 Ωcm, (100) orientation, 200 µm thick, planar surface) were RCA-cleaned and HF-dipped prior to deposition process. TiO_x was deposited by an ALD system (FlexAL, Oxford Instruments) on the rear-side of c-Si wafer. Titanium isopropoxide (TTIP) was used as a Ti precursor. The oxidation during every ALD cycle took place using either O_2 plasma or thermal reaction with H_2O vapor. We term these processes as plasma- and thermal-ALD, respectively. Although a substantially longer purge time was required after H_2O dose (30 s) than after O_2 plasma (2 s), TiO_x were deposited at a similar growth rate per cycle of ~0.045 nm in both ALD processes. In this study, to focus on the carrier selectivity of TiO_x, an intrinsic a-Si:H buffer layer (8-15 nm) was deposited by plasma-enhanced chemical vapor deposition prior to TiO_x. This buffer layer preserves the surface passivation quality unchanged regardless of the ALD condition, as confirmed by measuring the quasi-steady-state photoconductance (QSSPC) [10] before and after TiO_x deposition. As a rear contact after ALD-TiO_x, four different conductive materials (Ti, Al, Pd, and ITO) were examined. The front-side emitter or front-surface-field (FSF) was formed using a standard heterojunction structure (a-Si:H *i-p* or *i-n* stack), following a sputtered ITO layer [4]. As shown in Fig. 1, TiO_x acts either as electron contact and back-surface-field (BSF) or hole contact and rear-emitter for N-type base. Suns-V_{oc} measurement [11] was carried out before and after hotplate annealing at 180°C for 15 min in ambient air. Apart from solar cell precursors, TiO_x layers were directly

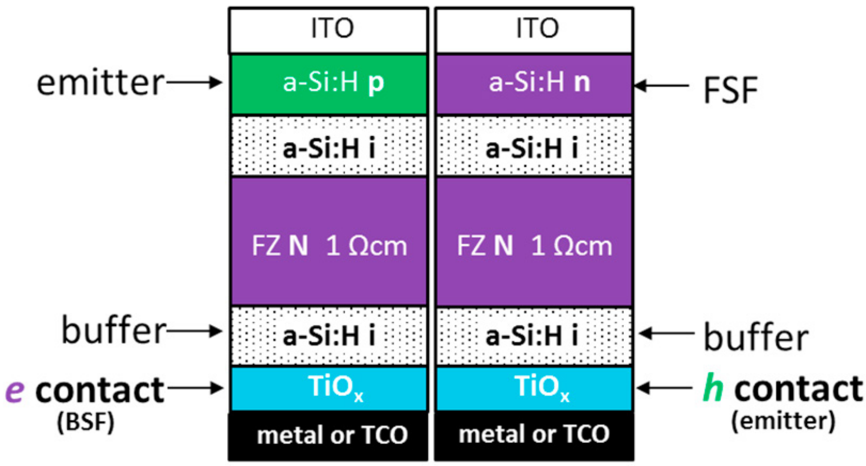

Fig. 1. Schematic illustration of sample structures studied in this work.