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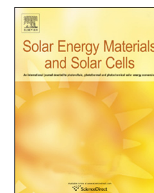

Explorative studies of novel silicon surface passivation materials: Considerations and lessons learned

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ABSTRACT

Despite the existence of several highly effective and well-characterized passivating materials for crystalline silicon surfaces, the topic of surface passivation and the investigation of new passivating materials remain of considerable interest for silicon photovoltaics research. However, the question of whether and under what circumstances a particular material will provide effective surface passivation remains difficult to answer. In this work, we provide an overview of recent insights relating to this question, drawing from our own work on novel passivation materials including MoO_x, Nb_2O_5, TiO_x, ZnO, and PO_x, and illustrated with experimental results. Factors that strongly influence the passivation performance include the use of pre-grown interfacial oxides, the film thickness, the annealing conditions, and the presence of capping layers. The impact of these factors on the surface passivation can vary widely from material to material. Therefore, all of these factors should be taken into account when investigating potential new surface passivation materials.

1. Introduction

Effective surface passivation is critical to realizing high-efficiency crystalline silicon (c-Si) solar cells and is becoming ever more important as wafer thicknesses are reduced and bulk Si quality improves. At the same time, new demands on the functionality of passivation layers have emerged, such as the ability to form passivating contact structures that in addition to passivation, enable the selective extraction of either positive or negative charges from the Si bulk [1,2]. These demands have stimulated significant research efforts aimed at evaluating the passivation properties of novel materials [1–9]. As a result, in the last decade, the list of materials known to be capable of effectively passivating c-Si surfaces has expanded significantly. The well-established Si-based passivation layers (SiO_2 [10], SiN_x [11], a-Si:H [12], and more recently proven Al_2O_3 [13–16]) have been joined by a range of new materials including HfO_2 [15,17,18], TiO_x [19–23], Ta_2O_5 [24] and Ga_2O_3 [25–27], and new passivation materials continue to be reported, such as ZnO [28], Nb_2O_5 [29, 84], PO_x [30,85], and ZrO_x [31]. Table 1 gives a summary of state-of-the-art passivation results for these materials and a few other notable examples. Note that some of these passivation materials can also serve as passivating contacts, as apart from preventing minority carrier recombination at the c-Si surface, they also yield a sufficiently low contact resistance to c-Si for majority carriers. In Fig. 1, transmission electron microscopy (TEM) images for a selection of these passivating materials are shown.

The mechanism of surface passivation is generally understood to involve a reduction in the number of interface states (“chemical” passivation) and/or suppression of the concentration of either electrons or holes at the semiconductor surface (historically referred to as “field-effect” passivation) (in general, effective passivation almost always involves a combination of these two mechanisms). However, the reasons for when and why a particular material will provide passivation are still not entirely clear. Some materials that were long believed not to provide effective surface passivation have now been shown to do so under the right conditions. For instance, TiO_x was replaced by SiN_x as the preferred anti-reflection coating (ARC) for c-Si solar cells in the late 1990s due to the more effective passivation provided by SiN_x, but it has recently been shown that TiO_x can in fact also provide excellent passivation [19–23]. On the other hand, other materials that are potentially relevant to c-Si photovoltaics thus far do not seem to provide passivation, regardless of their preparation method and post-deposition treatment. However, the growing number of studies of different

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Table 1
Selection of state-of-the-art passivation results reported for various passivation materials on *n*-type substrates with a bulk resistivity in the range of 1–7 Ω cm (unless otherwise specified). $S_{eff,max}$ values are calculated from the original lifetime data assuming an infinite bulk lifetime. In general we have selected the references with the lowest reported $S_{eff,max}$ in this resistivity range, giving preference to reports on more highly doped substrates in case of similar values. Representative values for the bandgap are given (additional references for these bandgap values have been included in cases where these are not mentioned in the reference for $S_{eff,max}$). The typical polarity (*n* or *p*) of the induced silicon space-charge region is specified. n^+ or p^+ indicate particularly strong band bending in the silicon, while *p*/*n* indicates that band bending is tunable through doping. We also specify the passivation layer thickness and whether a pre-grown SiO_x interlayer (either thermally or chemically grown) was present. Materials that are capable of forming passivating contacts for electron or holes are indicated.

Material	Bandgap (eV)	$S_{eff,max}$ (cm/s)	Induced surface charge	Preparation Method	Pre-grown SiO_x	Thickness (nm)	Remarks	Ref.
SiO_2	9[a]	2.4	*n*	Thermal oxidation	–	~ 110		[32]
SiN_x	1.8–5.3[a]	3.5	n^+	PECVD	–	> 50	Common ARC/passivation for n^+ Si in homojunction cells	[33]
a-Si:H	1.6–1.8	0.7	*p*/*n*	PECVD	–	280	*p*- or *n*-doping possible Can form e- or h-contact	[34]
poly-Si	~ 1.1[a]	0.4	*p*/*n*	LPCVD	therm.	150	*p*- or *n*-doping possible Can form e- or h- contact	[35]
Al_2O_3	6.4[a]	1.3	p^+	ALD	–	30	Common passivation for p^+ Si in PERC cells	[36]
PO_x	> 5	2.7	n^+	ALD	–	6		[30]
HfO_2	5.3–5.7	3.3	*n*	ALD	–	15		[18]
Ta_2O_5	4.4[a]	6.1	*p*	ALD	–	12		[24]
TiO_x	3.5	3.7	*p*	ALD	–	15	Former use as ARC. Can form e-contact	[21]
Ga_2O_3	4.2–5.2	6.4	p^+	ALD	–	4.5		[25]
MoO_x	2.8	29	p^+	ALD	chem.	10	Can form h-contact with a-Si:H	This work
Nb_2O_5	3.6	6.8	p^+	ALD	chem.	5	Can form e-contact	[29]
AlN	6.2	12[b]	*p*	Sputtering	chem.	50		[37]
ZnO	> 3	8.5	*n*	ALD	chem.	73	Common TCO, *n*-doping possible	[28]
ZrO_x	5–6	9.1	*p*	ALD	–	20		[31]

(ARC = Anti-reflection coating; TCO = Transparent conductive oxide).
[a] Values taken from Ref. [1] for SiO_2, poly-Si, and Ta_2O_5, Ref. [38] for SiN_x, and Ref. [16] for Al_2O_3.
[b] Obtained on 1 Ω cm *p*-type Si.

materials means that significantly more data relating to this question are becoming available.

In our group, we have investigated a large number of materials prepared by atomic layer deposition (ALD) for surface passivation of c-Si. ALD provides distinct advantages for surface passivation studies, such as large-area uniformity, precise thickness control, and damage-free ('soft') deposition [7]. Materials that have recently been examined include Nb_2O_5, PO_x, ZnO, TiO_x, and MoO_x. In this work, we will highlight several trends and exemplary cases taken from these and other datasets which provide insight into the factors that are important to surface passivation, with a particular emphasis on results that deviate from or go beyond conventional wisdom. While such examples do not yet permit us to outline a step-by-step procedure for reliably achieving surface passivation with new materials, they do highlight some important factors that ought to be taken into account when investigating novel materials for surface passivation properties. In particular we will highlight the role of pre-grown interfacial oxides (prepared by e.g. a standard Radio Corporation of America (RCA) clean or a low-temperature oxidation), the existence of different optima for film thickness, variation in optimum annealing temperature between different materials, and the potential role of capping layers in providing hydrogen for interface passivation. Since there are already a number of recent works which review passivating materials and/or passivating contacts [1–9], this work is not intended as a fully exhaustive review paper, but is instead primarily focused on providing the latest insights taken from a variety of relatively new passivation materials.

2. Experimental

As substrates for the ALD films discussed in this study we used double-side-polished (100) 1–5 Ωcm *n*-type floatzone (FZ) Si wafers. Films were deposited by ALD in Oxford Instruments FlexAL (in case of Nb_2O_5 [29], TiO_x [43], and Al_2O_3 [44]) or OpAL (in case of MoO_x [42,45] and H, Al or B doped ZnO [46-48]) reactors. Annealing was performed using a Jipelec rapid thermal annealing system. The passivation quality was assessed by transient and quasi-steady-state photoconductance (QSSPC) measurements using a Sinton WCT-120TS lifetime tester. Film thickness was evaluated using a J.A. Woollam M2000U variable angle spectroscopic ellipsometer.

3. Results

3.1. Surface preparation and the role of pre-grown interfacial oxides

The conventional silicon surface preparation procedure prior to surface passivation involves one or several wet-chemical cleaning steps (e.g. a Radio Corporation of America (RCA) standard clean [49]) which typically results in the growth of a thin (1–2 nm) surface oxide. Immediately before the deposition of a passivating film, this oxide is removed by etching in dilute hydrofluoric acid (HF) to leave a hydrophobic, hydrogen-terminated surface. The latter is generally considered the ideal starting surface for passivation, as such low-temperature wet chemical oxides are generally regarded as being of low-quality — usually they provide negligible passivation on their own — and their removal enables the formation of a new high-quality interface. This is well-established for example for thermal SiO_2 [50], PECVD SiN_x [51] and PECVD a-Si:H [34]. Note that, at least in the case of oxide materials, the formation of this new interface generally involves the growth of a new interfacial SiO_x layer either during deposition or upon subsequent annealing, (as visible in the TEM images shown in Fig. 1 of Al_2O_3, TiO_x, and Nb_2O_5 deposited on HF-treated Si), where the thickness and other properties of this layer will depend on the specific processing conditions and interfacial chemistry.

Contrary to this picture, we have found that in some cases retaining the oxide grown during surface cleaning, or intentionally growing a thin chemical oxide, can be beneficial for surface passivation by metal

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