

# Atomic-layer deposited Nb<sub>2</sub>O<sub>5</sub> as transparent passivating electron contact for c-Si solar cells

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## ABSTRACT

Passivating contacts based on metal oxides have proven to enable high energy conversion efficiencies for crystalline silicon (c-Si) solar cells at low processing complexity. In this work, the potential of atomic-layer deposited (ALD) Nb<sub>2</sub>O<sub>5</sub> as novel electron-selective passivating contact is explored in terms of recombination parameter  $J_0$  and contact resistivity  $\rho_c$ . It is shown that after forming gas annealing, ALD Nb<sub>2</sub>O<sub>5</sub> can provide adequate surface passivation with  $J_0$  values down to 25–30 fA/cm<sup>2</sup>. On HF-treated c-Si surfaces a minimum film thickness of ~ 3 nm is required to achieve this high level of passivation, whereas on surfaces with a wet-chemical SiO<sub>2</sub> interlayer the high passivation level is persistent down to film thicknesses of only 1 nm. Ohmic *n*-type contacts have been achieved using Al as contacting metal, where annealing the samples after Al contacting proved crucial for obtaining good contact properties. Low contact resistivity values of 70 and 124 mΩ cm<sup>2</sup> for 1 and 2 nm Nb<sub>2</sub>O<sub>5</sub> films, respectively, have been achieved on c-Si substrates that received an HF treatment prior to Nb<sub>2</sub>O<sub>5</sub> deposition. Transmission electron microscopy imaging shows that on such surfaces the annealing treatment leads to the formation of a (1.7 ± 0.2) nm interfacial oxide in between the c-Si substrate and the Nb<sub>2</sub>O<sub>5</sub> film. The presented results demonstrate the potential of ALD Nb<sub>2</sub>O<sub>5</sub> as electron-selective passivating contact and directions for future research are outlined.

## 1. Introduction

Passivating contacts have in recent years proven to be vital building blocks for high-efficiency crystalline silicon (c-Si) solar cells [1,2]. Passivating contacts, which typically consist of a stack of nanolayers, form the electron- and hole-selective contacts to silicon by (i) effectively passivating the c-Si surface, and by (ii) exhibiting a strong asymmetry in the conduction for electrons and holes, with the conductivity for the majority carrier (i.e., the carrier to be extracted) being sufficiently high [3]. These two requirements are met if [1,4]:

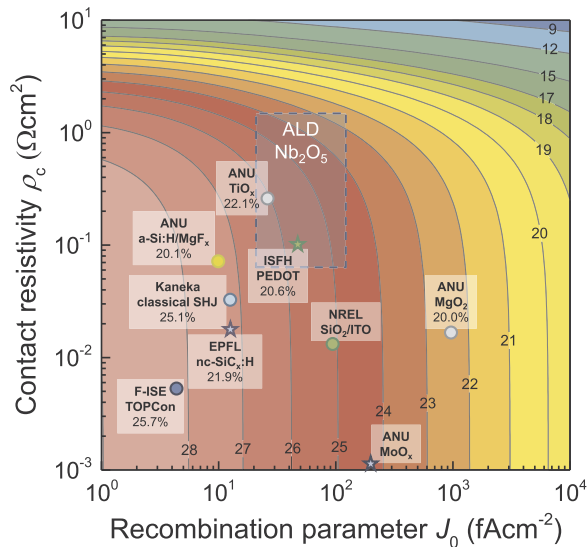
- A low surface recombination parameter  $J_0$  is measured, since this implies a well-passivated surface. If the  $J_0$  remains low after metallization, it means that at least one carrier type is shielded from the metal contact, since otherwise strong recombination would occur at the metal contact.
- A low contact resistivity  $\rho_c$  is measured, which implies that at least one carrier type can reach the metal contact without excessive Ohmic losses.

Although there are some caveats to using solely  $J_0$  and  $\rho_c$  to assess the electrical performance of a passivating contact (see e.g. Ref. [5]), it is a useful and facile way of assessing the efficiency potential. The influence of  $J_0$  and  $\rho_c$  on the simulated efficiency potential of an otherwise ideal c-Si solar cell is shown in the contour plot of Fig. 1, adapted from reference [1]. As can be seen, a lower  $J_0$  contributes strongly to a higher efficiency, mainly by an increase in open-circuit voltage  $V_{oc}$ , whereas a  $\rho_c$  below ~ 0.3 Ω cm<sup>2</sup> is required to prevent Ohmic losses from adversely affecting the fill factor.

As can also be seen in Fig. 1, passivating contacts based on stacks of intrinsic and doped amorphous silicon (i.e. classical silicon heterojunction (SHJ)) [6], as well as contacts based on ultrathin SiO<sub>2</sub>/doped poly-Si (often coined TOPCon [7] or POLO [8]), have been the most successful both in terms of  $J_0$  and  $\rho_c$  as well as efficiency. Although the success of these two approaches is hard to dispute, these doped Si materials do suffer from a relatively low optical transparency [9–11]. As such, the highest cell efficiencies of over 26% for these types of contacts have been reached using the more complex interdigitated back contact (IBC) structures [6,12]. In addition, the limited thermal

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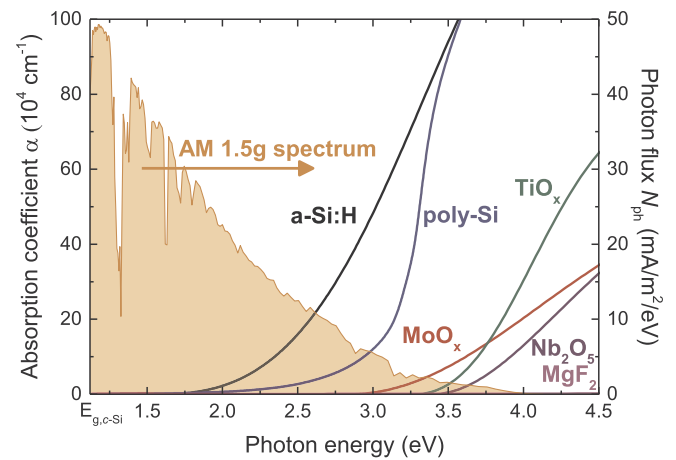


**Fig. 1.** Contour plot of the maximum attainable efficiency for an idealized *c*-Si solar cell as obtained from Quokka simulations. This figure has been adapted from reference [1]. The dashed rectangular region represents the range of  $J_0$  and  $\rho_c$  values reported for ALD  $\text{Nb}_2\text{O}_5$  in this work. Literature values of various passivating contact schemes and corresponding record efficiencies and affiliations are displayed. Electron- and hole-selective contacts are denoted by circular and star-shaped symbols, respectively.

stability of *a*-Si:H, and especially *p*-type *a*-Si:H, render SHJ cells incompatible with fire-through metallization schemes and conventional pastes [13,14].

These considerations have warranted the search for alternative carrier-selective materials, with the goal of finding materials that exhibit e.g. higher transparency or higher stability [15]. Many of the recently-explored materials are either metal oxide- or metal fluoride-based passivating contacts, with notable examples being  $\text{TiO}_x$  [16–18],  $\text{MgO}_2$  [19],  $\text{MoO}_x$  [20–22],  $\text{WO}_x$  [23–25],  $\text{V}_2\text{O}_5$  [23,26],  $\text{LiF}$  [27,28], and  $\text{MgF}_2$  [29]. Rather than relying on heavy doping, these more novel materials mostly achieve asymmetric carrier conductivity through other physical principles such as induced band bending arising from work function differences or suitable band offsets to *c*-Si [1,3,5,30]. As Fig. 1 also shows, these more novel approaches typically do not yet yield as good  $J_0$  and  $\rho_c$  values as doped *a*-Si:H and poly-Si. Yet, due to their higher band gap these materials do have the advantage of enhanced transparency. This is shown in Fig. 2, where the spectral absorption coefficient of a selection of these materials, as well as those of *a*-Si:H and poly-Si, are compared to  $\text{MoO}_x$ ,  $\text{TiO}_x$  and  $\text{MgF}_2$ . ALD  $\text{Nb}_2\text{O}_5$ , the material of this study, has been added. The refractive index  $n$  and extinction coefficient  $k$  of ALD  $\text{Nb}_2\text{O}_5$  can be found in Fig. S1 of the Supplementary information. As can be seen, the metal oxide- and metal fluoride-based contacts clearly provide higher transparency. This stems from their higher band gaps, which are 2.9, 3.3, 3.4 eV for ALD  $\text{MoO}_x$ ,  $\text{TiO}_x$  and  $\text{Nb}_2\text{O}_5$ , respectively, and 10.8 eV for  $\text{MgF}_2$  [31,32]. Besides the benefit of enhanced transparency, some of the novel materials can potentially lead to solar cell processing simplifications, as these very thin materials can often be deposited by atmospheric pressure deposition processes such as spatial ALD, which has already found its way into high-volume solar cell manufacturing [33].

In this work,  $\text{Nb}_2\text{O}_5$  prepared by ALD is explored as a novel electron-selective passivating contact material. As will become clear from this work, there are very strong similarities between ALD  $\text{Nb}_2\text{O}_5$  and  $\text{TiO}_x$ , both in terms of their material and contacting properties, as well as in their history in solar cells. Historically,  $\text{TiO}_x$  has been a commonly-employed antireflection coating in *c*-Si solar cells due its suitable refractive index and low optical absorption [38]. However, since  $\text{TiO}_x$  was not known for its ability to passivate the *c*-Si surface (and bulk) it



**Fig. 2.** Absorption coefficient ( $\alpha$ ) spectra for various common carrier-selective materials and for ALD  $\text{Nb}_2\text{O}_5$ . The AM1.5G solar spectrum is shown for reference. This figure has been adopted from Refs. [1,34], where data on *a*-Si:H [9], poly-Si [10],  $\text{MoO}_x$  [35],  $\text{TiO}_x$  [36] and  $\text{MgF}_2$  [37] were taken from literature. Note that the absorption coefficient of  $\text{MgF}_2$  is so low that it can hardly be seen on this scale.

was replaced by  $\text{SiN}_x$  in the early 1990s [39]. In addition,  $\text{TiO}_x$  is a common building block in organic and perovskite-based solar cells, where it is used as electron transport layer (ETL) due to its favorable band alignment with the absorber material [40,41]. The interest from the *c*-Si community was regained when Avasthi et al. demonstrated that  $\text{TiO}_x$  can also form an electron-selective contact to *c*-Si arguably due to its low conduction band (CB) and high valence band (VB) offsets [30]. However, the efficiency of 7% was not state-of-the-art, and most likely limited by a lack of surface passivation. One year later, it was demonstrated by Liao et al. that  $\text{TiO}_x$  prepared by ALD can actually yield a high level of surface passivation [16]. The passivation level was shown to improve through light-soaking, which was tentatively attributed to an increased negative charge density  $Q_f$  by charge injection [16]. From then on, there has been a stark and rapid increase in efficiency of these contacts up to 22.1% nowadays [17]. It was shown by TEM imaging that the Al overlayer, plays a key role in forming the contact by drawing oxygen from the  $\text{TiO}_x$  layer [42]. Further improvements to the contact have been enabled by using a tunnel  $\text{SiO}_2$  layer grown by thermal oxidation (TO) for passivation [17,18], and contacting by low work-function metals to improve the downward band bending [43]. Besides yielding a respectable efficiency at low processing complexity, these contacts have also been shown to be quite thermally stable during firing, albeit under slightly milder firing conditions [17].

Although not as common as  $\text{TiO}_2$ ,  $\text{Nb}_2\text{O}_5$  has also been used both as ARC in *c*-Si solar cells [44] and as ETL in perovskite solar cells [45,46] due to its very similar optical properties and band offsets as  $\text{TiO}_x$ , respectively. We have recently demonstrated that ALD  $\text{Nb}_2\text{O}_5$  can also very effectively passivate *c*-Si [47]. Part of the effective surface passivation was attributed to a negative fixed charge density of  $1\text{--}2 \times 10^{12} \text{ cm}^{-3}$ . Also, as was the case for  $\text{TiO}_x$ , the passivation of  $\text{Nb}_2\text{O}_5$  could be further enhanced by light-soaking, and the use of a thin wet chemically-grown  $\text{SiO}_2$  layer proved beneficial for the passivation performance.

In this work, the potential of ALD  $\text{Nb}_2\text{O}_5$  as passivating electron-selective contact for *c*-Si is explored. This is motivated by the use of  $\text{Nb}_2\text{O}_5$  as ETL in perovskite cells, as well as the reported electron affinity values of  $\text{Nb}_2\text{O}_5$  that lie in a typical range of 3.9–4.3 eV [48–50], which is very similar to the electron affinities of  $\text{TiO}_2$ , which are reported to be  $\sim 4$  eV [50]. Moreover, Hoffeditz et al. have recently directly compared the conduction band position of ALD  $\text{TiO}_2$  and ALD  $\text{Nb}_2\text{O}_5$ , using the same ALD precursor as in this work [51]. They found a small conduction band edge difference of 150 meV in the as-deposited state, which reduced to only 40 meV after annealing at 500 °C.

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