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Aluminum oxide-aluminum stacks for contact passivation in silicon solar cells

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Abstract

We investigate passivation of the aluminum-silicon interface by thin aluminum oxide (Al$_2$O$_3$) layers grown by thermal atomic layer deposition (ALD) on HF-last silicon surfaces. We first report effective lifetimes of Al$_2$O$_3$-passivated n- and p-type silicon wafers as a function of the number of ALD cycles. Then, we present saturation current density and contact resistance measurements of aluminum contacts on n/n$^+$ and n/p$^+$ junctions, passivated with a selection of the investigated layers. Our results show that aluminum contacts on n$^+$ silicon can be successfully passivated with thin Al$_2$O$_3$ layers without compromising contact resistance. However, we did not observe significant contact passivation for acceptable contact resistance in the case of Al$_2$O$_3$ passivated aluminum contacts on p$^+$ silicon. We explain our experimental results from the asymmetry between conductance and valence band offsets of Al$_2$O$_3$ on silicon.

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1. Introduction

Contact passivation is one of the enablers of highly efficient crystalline silicon solar cells, e.g. [1]. Thin dielectric layers are at the heart of the metal–(poly-Si)–insulator–semiconductor route for contact passivation and have been actively investigated in the context of silicon photovoltaics, e.g. [2]. Thicknesses of dielectrics $t_{ox}$ used for Ohmic contact passivation must be sufficiently low since, setting aside resonant tunneling effects, the transfer coefficient for tunneling through a barrier decreases exponentially with barrier thickness and height [3]. However, effective surface recombination velocities $S_{eff}$ of surfaces passivated with such thin layers decrease strongly with layer thickness. Therefore, a trade-off exists between contact passivation and contact resistance.

In this work, we investigate the passivation of the silicon-aluminum interface by thin aluminum oxide (Al$_2$O$_3$) layers for aluminum contacts on n$^+$ and p$^+$ silicon. We choose aluminum as a metal because it is a fairly benign impurity in silicon, it is abundant, and it has good infrared reflectivity. We investigate Al$_2$O$_3$ because it has proven to efficiently passivate aluminum contacts on n$^+$ Si without compromising contact resistance [2,4]. The Al$_2$O$_3$-Al stack we investigate can either be used as a contact itself, or as part of a contact stack comprising multiple metals. Note that an unavoidable thin SiO$_x$ layer is present between Si and Al$_2$O$_3$, see e.g. [5,6], which is part of the passivating stack.

### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
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<tbody>
<tr>
<td>ALD</td>
<td>atomic layer deposition</td>
<td></td>
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<tr>
<td>cTLM</td>
<td>circular transmission line method</td>
<td></td>
</tr>
<tr>
<td>$J_{0,\text{det}}$</td>
<td>saturation current density of junctions outside contacted regions</td>
<td>$[\text{fA} \cdot \text{cm}^2]$</td>
</tr>
<tr>
<td>$J_{0,\text{met}}$</td>
<td>contacted junction saturation current density</td>
<td>$[\text{fA} \cdot \text{cm}^2]$</td>
</tr>
<tr>
<td>$N_D$</td>
<td>bulk doping level</td>
<td>$[\text{cm}^{-3}]$</td>
</tr>
<tr>
<td>$n_i$</td>
<td>intrinsic concentration</td>
<td>$[\text{cm}^{-3}]$</td>
</tr>
<tr>
<td>$q$</td>
<td>elementary charge</td>
<td>$[\text{C}]$</td>
</tr>
<tr>
<td>$S_{eff}$</td>
<td>effective surface recombination velocity</td>
<td>$[\text{cm} \cdot \text{s}^{-1}]$</td>
</tr>
<tr>
<td>$t_{ox}$</td>
<td>tunnel barrier thickness</td>
<td>$[\text{cm}]$</td>
</tr>
<tr>
<td>$W$</td>
<td>wafer thickness</td>
<td>$[\text{cm}]$</td>
</tr>
<tr>
<td>$\Delta p$</td>
<td>bulk excess carrier density</td>
<td>$[\text{cm}^{-3}]$</td>
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<tr>
<td>$\Delta E_{c}$</td>
<td>conductance band offset</td>
<td>$[\text{eV}]$</td>
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<tr>
<td>$\Delta E_v$</td>
<td>valence band offset</td>
<td>$[\text{eV}]$</td>
</tr>
<tr>
<td>$\rho_c$</td>
<td>specific contact resistance</td>
<td>$[\Omega \cdot \text{cm}^2]$</td>
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<tr>
<td>$\tau_b$</td>
<td>bulk lifetime</td>
<td>$[\text{s}]$</td>
</tr>
<tr>
<td>$\tau_{eff}$</td>
<td>effective lifetime</td>
<td>$[\text{s}]$</td>
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2. Experimental

We investigate the passivation of aluminum contacts on chemically polished <100> Czochralski (Cz) Silicon wafers using thin Al$_2$O$_3$ layers deposited by thermal atomic layer deposition (ALD). Shortly before Al$_2$O$_3$ ALD deposition, which is performed in a spatial ALD tool, the wafers received a 10s dip in a diluted HF:HCl solution. All Al$_2$O$_3$ passivated samples received an anneal in N$_2$ at 500°C for 30 min before metal deposition.

We first extract effective lifetimes, $\tau_{eff}$, and oxide thickness, $t_{ox}$, as a function of the number of ALD cycles. $\tau_{eff}$ is used as a proxy for $S_{eff}$, the effective surface recombination velocity. $S_{eff}$ and $t_{ox}$ are used as rough indicators for contacted junction saturation current density, $J_{0,\text{met}}$, and contact resistance, $\rho_c$, respectively.

We measure $\tau_{eff}$ using quasi steady state photo conductance (QSSPC) measurements at 23°C. Effective lifetimes were measured on 160-170 μm thick, chemically polished, n- and p-type Czochralski silicon wafers passivated with thin Al$_2$O$_3$ passivation layers on both sides. The resistivity of the p-type layers was $\approx 2 \Omega \cdot \text{cm}$, the resistivity of the n-type wafers was between 0.8 and 5 $\Omega \cdot \text{cm}$. Bulk lifetime $\tau_b$ of these wafers is at least 800μs for the p-type wafers and 1200 μs for the n-type wafers, at an injection level of $1 \cdot 10^{15} \text{cm}^{-3}$. Therefore, $\tau_b$ is at least two times higher than
the observed $\tau_{\text{eff}}$ of Al$_2$O$_3$ passivated wafers such. As a result, the $\tau_{\text{eff}}$ shown in figure 1 are good measures for $S_{\text{eff}}$.

We use single wavelength ellipsometry at a wavelength of 633 nm for thickness measurements on mirror polished boron doped Czochralski silicon wafers with a resistivity higher than 1 Ω · cm. The index of refraction of as-grown Al$_2$O$_3$ layers under investigation is taken to be 1.62, which is a result obtained from ellipsometry on thick Al$_2$O$_3$ layers. All thickness measurements were done with the purpose of getting a rough estimate of the thicknesses of our layers. The thicknesses were extracted assuming that the only layer between silicon and the atmosphere was Al$_2$O$_3$, which is evidently an approximation since we did not take into account the thin SiO$_x$ layer between Al$_2$O$_3$ and silicon. However, since the index of refraction of quartz is 1.54 at 633 nm [7], we estimate that the relative error on the dielectric stack’s physical thickness that results from making this approximation is less than 5%, even if the entire stack would consist of SiO$_2$ instead of Al$_2$O$_3$.

Based on these $S_{\text{eff}}$ and $t_{\text{oxx}}$ results, $J_{0,\text{met}}$ and $\rho_c$ are measured for contacts passivated with a selected number of ALD cycles. $J_{0,\text{met}}$ and $\rho_c$ are measured on chemically polished n-type Cz silicon wafers. They received a B or P diffusion step and a thermal oxidation, forming passivated junctions on both sides. Then, test structures for $J_{0,\text{met}}$ measurement based on lattices of point contacts with varying pitch were made according to [8]. At each injection level, $J_{0,\text{met}} - J_{0,\text{diel}}$ was extracted from the slope of inverse effective lifetime as a function of the contact fraction $C_{\text{met}}$:

$$\frac{1}{\tau_{\text{eff}}} = \frac{1}{\tau_b} + 2 J_{0,\text{diel}} \frac{N_{bD} + \Delta p}{q \eta_i W} + C_{\text{met}} \frac{J_{0,\text{met}} - J_{0,\text{diel}}}{q \eta_i W}$$

in which all symbols have been defined in the table above. Point contact size and spacing were made small such that injection level variations within the wafer plane are small. We used high lifetime wafers and relatively low contact fractions to minimize injection level variations over the wafer thickness. Oxide openings and metal features were lithographically defined. Metal (sputtered Al:1%Si) thickness was 500 nm. A forming gas anneal at 400°C was done after contact lithography. Effective lifetime measurements were done at 23°C and the intrinsic carrier concentration was taken to be 7.4·10$^9$cm$^{-3}$ [9].

$\rho_c$ was measured using cTLM (circular Transfer Length Method) [10] measurements 25°C in all cases, except for the Al contact on p$^+$ silicon passivated with 9 ALD cycles, for which the transfer length was too large to be measurable with our particular cTLM structure. Therefore, we used an I-V measurement between one of the point contacts in the test structure for $J_{0,\text{met}}$ measurement and a much larger ohmic contact adjacent to the point contact. An optical micrograph of several point contacts and the ohmic contact is shown in figure 3(c). We neglected the resistance of the ohmic contact and the resistance of the p$^+$ silicon layer between ohmic contact and point contact. By comparison with a similar measurement on an unpassivated emitter contact, which has a much lower contact resistance, we estimate that the error we make by using this approximation is less than 10%. The data point shown for the contact resistance measurement on the p$^+$ contact passivated with 9 ALD cycles is the median value from 21 measurements and the indicated uncertainty is the interval between the maximum and minimum measured values. For the resistances measured using cTLM, the uncertainty on contact resistances was found from 95% confidence intervals on the transfer length and sheet resistance. We applied voltages below 5 mV in our contact resistance measurements. These low voltages are the relevant voltage range because excessive power loss due to contact resistance would occur if the voltage over the contacts under operating conditions were larger than a few millivolts. Therefore, contacting schemes are designed in practice such that the voltage drop over the contact is smaller than a few millivolts.

3. Effective lifetime and thickness measurements

Figure 1(a) shows effective lifetimes of Al$_2$O$_3$ passivated wafers as a function of the number of ALD cycles. Effective lifetimes strongly increase with the number of ALD cycles: effective lifetimes range from ca. 10 μs for 3 cycles to ca. 400 μs for 25 cycles. Remarkably, no significant difference in effective lifetimes was found between n- and p-type wafers passivated with the same number of ALD Al$_2$O$_3$ cycles. Since our n- and p-type wafers have about the same thickness and recombination in both types of wafers is dominated by surface recombination, this is a
clear indication that the surface recombination velocity is independent of doping type, for the specific case considered in our experiment. The results of our effective lifetime tests are consistent with observations made in the literature [11]. Note that this is a remarkable observation since Al₂O₃ is well known to be a negatively charged dielectric and highly asymmetric electron and hole capture cross sections have been reported for the Al₂O₃-Si interface [12]. It can be explained by acknowledging that even just the oxide charge density at the SiOₓ-Al₂O₃ interface (−4·10¹¹ cm⁻² [16]) is sufficient to cause inversion at the silicon surface of the lowly doped (ca. 10¹⁵ cm⁻³) n-type wafers (see e.g. [17]). The surface of the p-type wafers is in accumulation due to the negative oxide charge. Therefore, holes are the majority carriers at the dielectric-silicon interface for both n- and p-type wafers.

Figure 1(b) shows thicknesses of Al₂O₃ layers deposited on mirror polished p-Si surfaces shortly after an HF-dip, as a function of the number of ALD cycles. For a low number of ALD cycles, these thicknesses are significantly thicker than expected from steady state growth rate measurements on thick layers, which yield a steady state growth rate of 0.137 nm/cycle. Also, the relative thickness discrepancy is the highest for the thinnest Al₂O₃ layers. This can be explained by the well known presence of a thin SiOₓ layer between Al₂O₃ and silicon, see e.g. [5,6]. It could be formed either at room temperature in the atmosphere between HF dip and loading or while heating the wafers in the load lock of our ALD tool prior to deposition. Note that for ellipsometry measurements on silicon wafers immediately after an HF dip, an 0.6 nm thick layer was measured assuming the index of refraction used in our Al₂O₃ thickness measurements. Therefore, we cannot exclude a significant relative error for our thickness measurements of the thinnest Al₂O₃ layers.

4. Contact recombination

\[ J_{0,met} - J_{0,diel} \] was extracted at each injection level from a linear fit of inverse effective lifetime as a function of the contact fraction (equation 1). \( J_{0,met} - J_{0,diel} \) is shown in figure 2 as a function of injection level (Δp) for Al₂O₃:Al contacts with various numbers of ALD Al₂O₃ cycles. We used 95% confidence intervals of the slope of inverse lifetime versus injection level to calculate a measure for the statistical uncertainty in the \( J_{0,met} - J_{0,diel} \) measurement. Our estimate of this uncertainty varies between ±40 and ±100 \( fA \cdot cm^{-2} \), depending on the sample and on the injection level. Note that \( J_{0,met} - J_{0,diel} \) for the unpassivated BSF contact is lower than \( J_{0,met} - J_{0,diel} \) for the unpassivated emitter contact, and \( J_{0,diel} \) higher for the unpassivated BSF compared to the unpassivated emitter. This is explained from the fact that our BSF doping profile is deeper and has a higher surface concentration than our emitter doping profile.
Figure 2(a) shows $J_{0,\text{met}} - J_{0,\text{diel}}$ for Al$_2$O$_3$:Al contacts on a 45 $\Omega$/square n-n$^+$ junction (phosphorous doped), with a surface concentration of $3 \cdot 10^{19}$ cm$^{-3}$. $J_{0,\text{diel}}$ was smaller than 50 fA cm$^{-2}$. We observe a steady decrease of $J_{0,\text{met}} - J_{0,\text{diel}}$ with increasing numbers of ALD cycles for all injection levels, which indicates that the contact on n$^+$ silicon is effectively passivated.

Figure 2(b) shows $J_{0,\text{met}} - J_{0,\text{diel}}$ for Al$_2$O$_3$:Al contacts on a 100 $\Omega$/square n-p$^+$ junction (Boron doped), with a surface concentration of $1 \cdot 10^{19}$ cm$^{-3}$. For the emitter, $J_{0,\text{diel}}$ was less than 25 fA cm$^{-2}$. We do not observe decreasing emitter saturation current densities with increasing number of ALD cycles. In part, this may be explained by the asymmetrical band structure of the contact passivation layer, which we discuss in paragraph 6. However, it may also be partly be due to measurement errors related to current flow through the point contacts in the test structure, as explained below.

In the test structure we used for $J_{0,\text{met}}$ measurement, $J_{0,\text{met}}$ is underestimated when significant current flows through the point contacts during the QSSPC measurement [8]. This parasitic effect is avoided when the contact’s transfer length is (much) larger than the contact size. For our contacts on n$^+$ silicon, the transfer length ($>29\mu$m) was significantly larger than the diameter of the circular contacts (ca. 15$\mu$m), such that we do not expect saturation current density to be significantly underestimated. For our contacts on p$^+$ silicon, this effect is expected to be significant for the unpassivated contact ($L_T \approx 6\mu$m) and for the contact passivated with 5 ALD cycles ($L_T \approx 8\mu$m), and it is expected to be small for p$^+$ silicon contacts passivated with thicker Al$_2$O$_3$ layers ($L_T > 43\mu$m).

$J_{0,\text{met}} - J_{0,\text{diel}}$ seemingly decreases with injection level for all samples. This is likely to be a parasitic effect similar to the effect of non-uniform excess carrier profiles on saturation current density extraction on blanket test structures reported by Kane and Swanson [13]. In fact, it is straightforward to show that, for non-uniform excess carrier densities over wafer thickness, saturation current densities extracted using equation one are underestimated by the factor $p_n m_{\text{met}} / p_n m_{\text{av}}$, in which $p_n m_{\text{met}}$ is the pn product at the bulk side of the space charge region between contacted junction and bulk, and $p_n m_{\text{av}}$ is the pn product in terms of the average injection level. This ratio is expected to decrease with increasing injection levels since the effective surface recombination velocity that describes junction recombination increases with injection level. As a result, saturation current densities extracted using equation one seemingly decrease with injection level.

5. Contact resistance

In figure 3(a), we show contact resistance of Al$_2$O$_3$ passivated contacts on our emitter (p$^+$ Si) and BSF (n$^+$ Si). The unpassivated BSF contact has a higher contact resistance than the unpassivated emitter contact even though the
surface doping concentration is higher for the BSF than for the emitter. This is due to the higher Schottky barrier height of Al contacts on n⁺ Si compared to Al contacts on p⁺ Si. However, the contact resistance of BSF contacts increases much more slowly with the number of ALD cycles than the contact resistance of our emitter contacts. By comparison of figure 2 with figure 3, it is clear that ALD Al₂O₃ can provide very significant passivation of aluminum contacts on n⁺ silicon for a relatively minor increase in contact resistance. However, the presence of an ALD Al₂O₃ layer between Al and p⁺ Si quickly results in excessive contact resistance while providing at most limited contact passivation, as shown in figure 2(b).

Note that for most measurements, the uncertainty on emitter contact resistance is much higher than the uncertainty on BSF contact resistance. This is caused by the fact that for the unpassivated emitter contact and for the emitter contact passivated with 5 Al₂O₃ ALD cycles, contact resistance was very low such that it was difficult to measure using our particular cTLM test structure. For the passivated emitter contact with 9 ALD cycles, contact resistance was too high to be measurable using our particular cTLM structure and we used the I-V characteristics of a very small point contact for contact resistance measurement instead. This structure is shown in figure 3(c). There was a large spread on those I-V characteristics, which we suspect to be related to significant roughness on length scales larger than the small contact used in this particular measurement. Since roughness changes surface orientation, and since roughness introduces topological features such as microscopic ridges and valleys, it is plausible that it can locally affect contact properties. However, the roughness length scale is much smaller than the contacts used in the cTLM measurement, such that the influence of small surface features on contact resistance is averaged and does not cause much spread in contact resistance extracted from our cTLM measurements.

We analysed the temperature dependence of contact resistance at voltages below 5 mV between 25 and 100 °C (figure 3(b)) for two samples. These samples were chosen because they present a reasonable trade-off between contact resistance and contact passivation. It is clear that for these samples, contact resistance is not thermally activated within the precision of our measurements. This fact is consistent with current transport through the dielectric that is dominated by direct tunnelling through the SiOₓ/Al₂O₃ passivation layer. For small fields and thin oxides, the direct tunnelling transport mechanism is indeed expected (see e.g. [3] p. 438). This should be contrasted with the trap assisted tunnelling mechanism that has been found to be dominating at low operating voltages in (thicker) high-κ gate dielectric stacks in the context of complementary metal oxide semiconductor (CMOS) devices [14]. Other transport mechanisms, notably Poole-Frenkel emission and Fowler-Nordheim tunnelling, are expected to be dominating at significantly larger electric fields, and for thicker oxides.

Fig. 3. (a) $\rho_c$ of Al₂O₃ passivated Al contacts on our BSF (n⁺ Si) and on our emitter (p⁺ Si), measured at 25°C. b) $\rho_c$ as a function of temperature for selected contacts. The thin dashed lines in figures 3 (a) and (b) indicate the uncertainty in the contact resistance measurement; (c) optical micrograph of the test structure used for measuring the emitter contact passivated with 9 ALD cycles.
6. Contact resistance versus contact recombination

Our experiments yield several key observations on the passivation of Al-Si interfaces using Al₂O₃ on HF-last Si. Firstly, \( I_{0,\text{met}} \) consistently decreases with increasing numbers of ALD cycles for passivated contacts on n⁺ silicon. However, we failed to observe appreciable contact passivation on p⁺ silicon. Secondly, \( \rho_c \) consistently increases with the number of ALD cycles for contacts on both n⁻ and p⁺ silicon. Finally, \( \rho_c \) increases much faster with the number of ALD cycles for p⁺ silicon compared to n⁻ silicon. We explain these experimental observations below.

The passivation effect of a thin dielectric layer between metal contact and semiconductor is due to two effects. Firstly, the silicon-metal interface is replaced by a silicon-dielectric interface, which reduces the density of states at the silicon surface, thereby reducing the surface recombination current. Secondly, the dielectric forms a barrier that shields minority carriers from the metal. This is also an essential effect since minority carrier flow from the semiconductor into the contact is effectively a recombination current. The transfer coefficient for tunnelling, i.e. the tunnelling probability, of carriers through a rectangular barrier is approximately given by [3] p. 440:

\[
T_t \approx \exp\left(-\frac{2d \sqrt{2q m^* \phi_F}}{\hbar}\right),
\]

in which \( d \) is barrier thickness, \( q \) is elementary charge, \( m^* \) is effective mass in the barrier, \( q \phi_F \) is effective barrier height in eV, and \( \hbar \) equals \( h/2\pi \), with \( h \) Planck’s constant. Also, we make the simplifying assumption that all electrons (holes) are situated at the top (bottom) of silicon’s conduction (valence) band. As a consequence and in the context of our passivated contacts, the barrier height for electron flow through the dielectric corresponds to the conductance band offset \( \Delta E_v \) between dielectric and silicon, and the barrier height for hole flow through the dielectric corresponds to the valence band offset \( \Delta E_c \) between dielectric and silicon.

The contact passivation layer under investigation is actually a SiOₓ:Al₂O₃ stack, since it is well known that a thin SiOₓ layer unavoidably grows between Al₂O₃ and silicon. The valence band offset \( \Delta E_v \) of SiO₂ on Si is 4.35 to 4.54 eV and the conductance band offset \( \Delta E_c \) of SiO₂ on Si is 3.15-3.5 eV. For Al₂O₃ on Si, \( \Delta E_v \) is 2.95-3.75 eV and \( \Delta E_c = 2.08-2.8 \) eV [5]. For the purpose of our qualitative reasoning, we disregard the fact that SiO₂ and Al₂O₃ have different band offsets, but we use the fact that for both SiO₂ and Al₂O₃, \( \Delta E_v > \Delta E_c \). Therefore, the tunnelling probability through the SiOₓ:Al₂O₃ stack is smaller for holes than for electrons, all other things equal.

\( \rho_c \) is determined by the resistance to majority carrier flow. In Al₂O₃-passivated contacts on silicon, resistance to the flow of holes from silicon to metal is bigger than the resistance to the flow of electrons from silicon to metal since \( \Delta E_v > \Delta E_c \). It therefore follows that contact resistance on our n⁺ BSF is expected to increase slowly with the number of Al₂O₃ ALD cycles compared to contact resistance on our p⁺ emitter. This corresponds to the experimental observation of contact resistance as a function of the number of Al₂O₃ ALD cycles, shown in figure 3(a).

The effective surface recombination velocity of the contact is determined by surface recombination at the Si-SiOₓ:Al₂O₃ interface, and by the tunnelling probability of minority carriers from the semiconductor to the metal. We assume that the effective surface recombination velocity at the Si-SiOₓ:Al₂O₃ interface is similar for both our emitter and back surface field, which is an assumption that is consistent with our effective lifetime measurements on lowly doped Al₂O₃-passivated n⁻ and p-type Si (figure 1(a)). As the Al₂O₃ layer thickness increases with the number of ALD cycles, the tunnelling probability of minority carriers through the SiOₓ:Al₂O₃ stack decreases with increasing numbers of ALD cycles. We suggest that this mechanism lies at the basis of the experimental observation that \( I_{0,\text{met}} \) consistently decreases with the number of ALD cycles for passivated contacts on our n⁻ BSF.

Since \( \Delta E_v > \Delta E_c \), the transmission coefficient through the barrier is smaller for holes than for electrons, and the resistance to minority carrier flow is larger for the passivated n⁻ BSF compared to the passivated p⁺ emitter, all other things equal. As a result, \( I_{0,\text{met}} \) of the passivated n⁻ BSF is expected to decrease faster with the number of ALD cycles than \( I_{0,\text{met}} \) of the passivated p⁺ emitter. This can in part explain why we observed consistently improving n⁻ BSF contact passivation with the number of ALD cycles, and we failed to observe such a trend for passivated contacts on our p⁺ emitter. However, measurement errors due to current flow through the point contacts instead of through the semiconductor may also be part of the explanation for the failure to detect contact passivation on our p⁺ emitter.

So far, our analysis did not consider the possibility of charged tunnel barriers even though the presence of fixed
negative charge in thicker Al₂O₃ layers is well known to play an important role in surface passivation by such thick Al₂O₃ layers, see e.g. [15]. The charge density was found to be $-4 \cdot 10^{11}$ cm$^{-2}$ elementary charges at the SiOₓ-Al₂O₃ interface and $-1 \cdot 10^{19}$ cm$^{-3}$ elementary charges in the Al₂O₃ layer [16]. The thickness of the layers we investigated was below 4 nm, which yields overall charge densities of $-4 \cdot 10^{11}$ to $-4.4 \cdot 10^{11}$ cm$^{-2}$. The fact that the overall surface charge density is not expected to change significantly with the number of ALD cycles for the samples we investigated is consistent with our contact resistance measurements: increasing negative charge density in a tunnel barrier would increase the Schottky barrier height for passivated n⁺ Si-Al contacts and it would decrease the Schottky barrier height for Al₂O₃ passivated p⁺ Si-Al contacts. Therefore, if the surface charge would increase significantly with the number of ALD cycles in the investigated range, contact resistance of Al₂O₃ passivated n⁺ Si-Al contacts would tend to increase faster with the number of ALD cycles than contact resistance of Al₂O₃ passivated p⁺ Si-Al interfaces. This contradicts our experimental observations, which motivates the interpretation of our experimental results in terms of band offsets and a reduction in surface states.

7. Conclusions

In conclusion, we investigated the applicability of thin thermal ALD Al₂O₃ layers deposited shortly after an HF-dip to the passivation of the interface between aluminum and n⁺ or p⁺ silicon. We find that for passivated aluminum contacts on n⁺ silicon, $J_{0,\text{net}}$ decreases with the number of ALD cycles and $\rho_c$ increases with the number of ALD cycles. We did not detect contact passivation of aluminum contacts on p⁺ silicon by ALD Al₂O₃. The increase of $\rho_c$ with the number of Al₂O₃ ALD cycles is much slower for Al contacts on n⁺ silicon compared to Al contacts on p⁺ silicon. Our results show that thin ALD Al₂O₃ layers on HF-last silicon can be an attractive technique for reducing recombination currents at the aluminum-n⁺ silicon interface. However, we did not observe passivation of the aluminum-p⁺ silicon interface for acceptable contact resistance. We explained our results qualitatively from the asymmetry of conductance and valence band offsets of Al₂O₃ and SiO₂ on silicon.

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