Silicon surface passivation by Al₂O₃: Recombination parameters and inversion layer solar cells

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Abstract

The interface between p- and n-type FZ-Si and an amorphous aluminum oxide (Al₂O₃) surface passivation layer deposited by plasma-assisted atomic layer deposition (ALD) was investigated by frequency-dependent conductance measurements. The hole capture cross section in the lower half of the bandgap, \( \sigma_p = (4 \pm 3) \times 10^{-16} \text{ cm}^2 \), was found to be independent of energy. The electron capture cross section \( \sigma_n \) in the upper half of the bandgap decreases from \( \sigma_n = (7 \pm 4) \times 10^{-15} \text{ cm}^2 \) at midgap over two orders of magnitude towards the conduction band edge. Numerical simulations of the effective surface recombination velocity based on these recombination parameters show a good agreement with experimental surface recombination velocities for a wide range of excess carrier and surface charge densities. Carrier transport in the inversion layer formed at the n-Si/Al₂O₃ interface was investigated yielding a sheet resistance of 15 kΩ/□, which was reduced to 6 kΩ/□ for a surface charge density of \( -2 \times 10^{13} \text{ cm}^{-2} \) obtained by corona charging. The applicability of Al₂O₃ inversion layers as emitters in n-type inversion layer solar cells was demonstrated by short circuit current densities of up to 25 mA/cm², which show a pronounced dependence on surface charge density.

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1. Introduction

Aluminum oxide (Al₂O₃) deposited by atomic layer deposition (ALD) provides an outstanding level of surface passivation on both n- and p-type crystalline silicon [1,2] and is an ideal choice for the surface
passivation of silicon solar cells [3,4]. A detailed knowledge of the energy-dependent electron-hole recombination parameters at the c-Si/Al₂O₃ interface enables highly predictive simulations of the interface recombination processes at the Al₂O₃-passivated solar cell surface, and hence would be of great benefit for the development and improvement of novel high-efficiency solar cells. In addition, an inversion layer forming at the surface of an n-Si wafer passivated with an Al₂O₃ film offers the opportunity to avoid a boron diffusion in the fabrication of n-type solar cells, as the inversion layer may act as charge collecting emitter in a novel n-type inversion layer solar cell as proposed in this contribution.

2. Interface recombination parameters

We measure the interface recombination parameters at the c-Si/Al₂O₃ interface as a function of the energetic position in the silicon bandgap using frequency-dependent conductance measurements [5] on metal-insulator-silicon (MIS) capacitors. The MIS-capacitors are fabricated on 1.3 – 1.5 Ωcm p-type and 1.5 Ωcm n-type FZ-Si wafers, respectively. The samples are coated on one side with 10 nm of Al₂O₃ deposited by plasma-assisted ALD. All samples are annealed for 15 min at 425 °C, then circular aluminum gate contacts are defined on top of the Al₂O₃ film by electron gun evaporation through a shadow mask, and a full-area aluminum back contact is evaporated on the non-coated side of the wafer. Figure 1(a) shows a sketch of the sample structure and the corresponding electric equivalent circuit. All relevant information about the interface recombination parameters is contained in the equivalent parallel conductance \( G_p \), which is the conductive component of the interface-trap-related admittance \( Y_{it} \) in Fig. 1(a). The total admittance \( Y_{ad}(\omega) \) is measured as a function of the angular frequency \( \omega \) at a fixed gate bias voltage \( V_G \) corresponding to a certain energetic position \( E_t \) in the silicon bandgap. Then \( G_p \) is extracted from \( Y_{ad}(\omega) \) and corrected for series resistance following a method described by Nicollian and Brews [6]. Figure 1(b) shows exemplary plots of the measured normalized parallel conductance \( G_p/\omega \) as a function of \( \omega \) for three different gate voltages \( V_G \).

Figure 2 shows the capture time constants \( \tau_p \) (below midgap, measured on p-type samples) and \( \tau_n \) (above midgap, measured on n-type samples), the corresponding capture cross sections \( \sigma_p \) and \( \sigma_n \), and the interface state density \( D_{it} \) deduced from the peak of \( G_p/\omega \) as function of \( \omega \) using the following relations:

![Fig. 1. (a) Sketch of the Al/Al₂O₃/Si capacitor (left) and corresponding electric equivalent circuit (right). (b) Exemplary plots of the normalized parallel conductance \( G_p/\omega \) as a function of angular frequency \( \omega \) for gate voltages of \( V_G = 0.35, 0.40, \) and \( 0.45 \) V on 1.5 Ωcm n-type FZ-Si for an Al₂O₃ film thickness of 10 nm.](image-url)
where $E_i$ is the intrinsic Fermi energy, $k_B$ is the Boltzmann constant, and $T$ is the temperature. A more detailed analysis of the data is presented in [7], a description of the method can be found in [6].

We obtain capture cross sections of $V_n = (7\pm4)\times10^{15}$ cm$^2$ and $V_p = (4\pm3)\times10^{16}$ cm$^2$ at midgap, which result in an asymmetry of $V_n/V_p = 5 - 70$. The hole capture cross section $V_p$ below midgap is virtually independent of energy, while the electron capture cross section $V_n$ above midgap decreases over two orders of magnitude towards the conduction band edge. It should be kept in mind, however, that small variations in the capture time constant lead to a large error in the capture cross section, which could conceal a more pronounced energy dependence of $V_p$.

The interface state density $D_{it}$ obtained by the conductance method is compared to $D_{it}$ values obtained by capacitance-voltage ($C-V$) analysis [8]. Both methods are in excellent agreement and yield a virtually constant $D_{it} = (6–20)\times10^{10}$ eV$^{-1}$cm$^{-2}$ near midgap with a small Gaussian-shaped peak around an energy of 0.9 eV above the valence band edge [solid green line in Fig. 2(c)]. The steep increase in $D_{it}$ towards the band edges shown in Fig. 2(c) is attributed to the impact of series resistance and inversion layer capacitance, which have been neglected in the analysis, and is hence neglected for numerical simulations.

3. Surface recombination velocity

We use an iterative numerical model presented by Girisch et al. [9], assuming flat quasi Fermi levels in the space charge region, and Shockley-Read-Hall (SRH) [10,11] theory to calculate the interface recombination velocity $S_i$ at the c-Si/Al$_2$O$_3$ interface as a function of excess carrier density $\Delta n$, given by the following equation [9,10]:

$$S_i = \left( \frac{n_i p_i - n_s^2}{\Delta n} \right) \int_{E_t}^{E_v} \left[ \frac{n_i + n_i(E_i)}{\sigma_n(E_i)} + \frac{p_i + p_i(E_i)}{\sigma_p(E_i)} \right] v_{iD}(E_i) dE_i,$$

where $n_i(E)$ and $p_i(E)$ are the energy-dependent SRH-densities for a defect level at energy $E_i$ [9], and $n_s$ and $p_s$ are the electron and hole concentrations at the interface. The resulting $S_i$ is then folded with a Gaussian distribution of the surface charge density $Q_z$ to account for spatial inhomogeneities of the field.
effect passivation. To verify the simulations we measure the effective carrier lifetime $\tau_{\text{eff}}$ as a function of excess carrier density $\Delta n$ on $p$- and $n$-type FZ-Si samples passivated on both sides with Al$_2$O$_3$ layers deposited by plasma-assisted ALD. The effective surface recombination velocity (SRV) $S_{\text{eff}}$ is then calculated from $\tau_{\text{eff}}$ using the equation [12]:

$$S_{\text{eff}} = \frac{w}{2} \left[ \tau_{\text{eff}} - \frac{w^2}{\pi D} \right]^{1/2} - \tau_b^{-1},$$

where $w$ is the wafer thickness, $D$ is the minority carrier diffusion constant, and $\tau_b$ is the bulk lifetime. For $\tau_b$ we use an empirical parameterization [13], which accounts for intrinsic radiative and Auger recombination. Further losses, e.g. recombination via bulk defects, are neglected. Hence we obtain an upper limit $S_{\text{eff,max}}$ of the surface recombination velocity.

The conductance method is only sensitive to majority carriers, and hence the capture cross sections $\sigma_p$ and $\sigma_n$ are only known in one half of the bandgap. We replace the unknown values of $\sigma_{n/p}$ by the midgap values of $\sigma_p$ and $\sigma_n$, as the choice of model only has a small effect on the calculated $S_{\text{eff}}$ [7].

Due to the excellent field-effect passivation caused by the high negative fixed charge density $Q_f = -(4\pm1) \times 10^{12}$ cm$^{-2}$ at the c-Si/Al$_2$O$_3$ interface [8], interface recombination is strongly suppressed. We gradually compensate $Q_f$ by corona charging, the total surface charge density $Q_6$ is then given by the sum of $Q_f$ and the deposited corona charge density $Q_c$. Figures 3(a) and (b) show the numerically calculated (lines) and experimentally determined (symbols) injection-level-dependent effective SRV $S_{\text{eff}}(\Delta n)$ for 1.3 $\Omega cm$ $p$-Si and 1.0 $\Omega cm$ $n$-Si, respectively, for different exemplary $Q_6$ values. The calculated $S_{\text{eff}}$ values include the interface recombination velocity $S_{\text{it}}$ and, in order to explain the injection level dependence of the lower plot ($Q_6 = 3.8 \times 10^{12}$ cm$^{-2}$, black line), an increased recombination in the space

Fig. 3. Calculated (lines) and experimentally determined (symbols) effective SRV $S_{\text{eff}}$ for (a) 1.3 $\Omega cm$ $p$-Si and (b) 1.0 $\Omega cm$ $n$-Si as a function of excess carrier density $\Delta n$ for different negative (closed symbols) and positive (open symbols) surface charge densities $Q_c$ given in the plot. The green dashed lines are calculated assuming an increased interface state density $D_{\text{it}}$, in order to account for interface damage induced during excessive corona charging. No error bar is given due to this assumption.
charge region [14,15]. At low \(|Q_6|\) values interface recombination dominates and recombination in the space charge region becomes negligible. The calculated \(S_{\text{eff}}(\Delta n)\) curves are in excellent agreement with the experimental data, taking into account that recombination via bulk defects has been neglected. However, we observe two exceptions: (i) For \(Q_6\) near zero, \(S_{\text{eff}}\) seems to be systematically overestimated, although calculation and experiment agree within the uncertainty. For \(Q_6\) near zero \(S_{\text{eff}}\) is sensitive to small changes in \(Q_6\) of the order of \(10^{11}\) cm\(^{-2}\), which is below the smallest charging step of \(\Delta Q_c \approx 5 \times 10^{11}\) cm\(^{-2}\) in our experimental setup. Hence, a slight deviation from \(Q_c = 0\) or assuming a larger inhomogeneity of the deposited corona charge is expected to lead to a better agreement. (ii) As previously shown in Ref. 7, \(S_{\text{eff}}\) is significantly underestimated for large values of \(Q_6 > +10^{12}\) cm\(^{-2}\). We attribute this to damage occurring during corona charging, as the same effect is observed for both \(p\)- and \(n\)-type samples, and hence is unlikely to be related to the charge polarity. This interpretation is supported by our experimental finding that after removal of the corona charges using deionized water the carrier lifetime is reduced compared to the initial lifetime of the sample. Assuming an increased interface state density \(D_{\text{it}}\), which we measured after degrading the c-Si/Al\(_2\)O\(_3\) interface by applying a large bias voltage [black diamonds in Fig. 2(c)], leads to a good agreement between calculated and experimental \(S_{\text{it}}\) values for \(Q_6 = +1.2 \times 10^{12}\) cm\(^{-2}\).

### 4. Inversion layer solar cell

Due to the negative fixed charge density at the c-Si/Al\(_2\)O\(_3\) interface, an inversion layer forms at the surface of an \(n\)-Si wafer passivated with an Al\(_2\)O\(_3\) film, which may be applied as emitter in \(n\)-type inversion layer solar cells. Figure 4(a) shows the sheet resistance \(R_{\text{cl}}\) of the inversion layer determined by the transition line method (TLM) as a function of surface charge density \(Q_6\), with values ranging from \(R_{\text{cl}} = 15\) k\(\Omega/\square\) for \(Q_6 = Q_f = -3.8 \times 10^{12}\) cm\(^{-2}\) down to 6 k\(\Omega/\square\) for \(Q_6 = -2 \times 10^{13}\) cm\(^{-2}\). For a contact spacing of 200 \(\mu\)m, these \(R_{\text{cl}}\) values correspond to a series resistance contribution of 0.2 – 0.5 \(\Omega\)cm\(^2\), sufficiently low to make an inversion emitter formed by Al\(_2\)O\(_3\) deposition feasible. Figure 4(b) shows a sketch of a 165 \(\mu\)m thick 2×2 cm\(^2\) inversion layer solar cell fabricated on 1 \(\Omega\)cm \(n\)-type Cz-Si with a non-optimized front finger spacing of 280 \(\mu\)m. The short circuit current density \(J_{\text{sc}}\) measured under standard test conditions (AM1.5G, 100 mW/cm\(^2\), 25 °C) is shown as blue squares in Fig. 4(a) as a function of \(Q_6\), yielding values of up to 25 mA/cm\(^2\). The pronounced dependence of \(J_{\text{sc}}\) on \(Q_6\) is strong evidence that the inversion layer is indeed acting as charge collecting emitter in the solar cell. Further experiments at our lab will reveal the full potential of Al\(_2\)O\(_3\)-induced inversion layers for \(n\)-type Si solar cells.

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**Fig. 4.** (a) Inversion layer sheet resistance \(R_{\text{cl}}\) determined by TLM (red circles) and short circuit current density \(J_{\text{sc}}\) measured under standard test conditions (AM1.5G, 100 mW/cm\(^2\), 25 °C) on 2×2 cm\(^2\) Al\(_2\)O\(_3\) inversion layer solar cells (blue squares) as a function of surface charge density \(Q_6\). The lines are guides to the eye. (b) Sketch of the Al\(_2\)O\(_3\) inversion layer solar cell fabricated on \(n\)-Si.
5. Conclusions

The interface between p- and n-type FZ-Si and an amorphous Al₂O₃ surface passivation layer deposited by plasma-assisted ALD was investigated by conductance measurements. The hole capture cross section in the lower half of the bandgap, \( \sigma_p = (4 \pm 3) \times 10^{-16} \text{ cm}^2 \), was found to be independent of energy. The electron capture cross section in the upper half of the bandgap on the other hand decreases from \( \sigma_n = (7 \pm 4) \times 10^{-15} \text{ cm}^2 \) at midgap over two orders of magnitude towards the conduction band edge \( E_c \). The capture cross section ratio at midgap is highly asymmetric with \( \sigma_n / \sigma_p = 5 – 70 \). The interface state density \( D_{it} \) shows an excellent agreement with values obtained from capacitance-voltage analysis, yielding \( D_{it} \) values around the middle of the bandgap of the order of \( 10^{11} \text{ eV}^{-1}\text{cm}^2 \). Numerical calculations of the injection level dependent surface recombination velocity based on these interface recombination parameters for Al₂O₃-passivated samples show a good agreement to experimental data for both n- and p-Si and for a wide range of surface charge densities. However, the interface quality is shown to degrade after deposition of large corona charge densities. We determine a sheet resistance of \( R_s = 15 \text{k}\Omega/\square \) for the inversion layer formed at the n-Si/Al₂O₃ interface, which was reduced to 6 k\( \Omega/\square \) by corona charging. We propose a novel n-type inversion layer solar cell, where the emitter consists of an inversion layer formed by depositing an Al₂O₃ layer on top of the n-type Si. We obtain short circuit current densities up to 25 mA/cm², which show a strong dependence on surface charge density, clearly demonstrating the feasibility of an n-type inversion layer solar cell formed by Al₂O₃ deposition.

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References