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Amorphous silicon enhanced metal-insulator-semiconductor contacts for silicon solar cells

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Carrier recombination at the metal-semiconductor contacts has become a significant obstacle to the further advancement of high-efficiency diffused-junction silicon solar cells. This paper provides the proof-of-concept of a procedure to reduce contact recombination by means of enhanced metal-insulator-semiconductor (MIS) structures. Lightly diffused n^+ and p^+ surfaces are passivated with $\text{SiO}_2/a\text{-Si:H}$ and $\text{Al}_2\text{O}_3/a\text{-Si:H}$ stacks, respectively, before the MIS contacts are formed by a thermally activated alloying process between the $a\text{-Si:H}$ layer and an overlying aluminum film. Transmission/scanning transmission electron microscopy (TEM/STEM) and energy dispersive x-ray spectroscopy are used to ascertain the nature of the alloy. Idealized solar cell simulations reveal that MIS(n^+) contacts, with SiO_2 thicknesses of $\sim 1.55\text{ nm}$, achieve the best carrier-selectivity producing a contact resistivity ρ_c of $\sim 3\text{ m}\Omega\text{ cm}^2$ and a recombination current density J_{0c} of $\sim 40\text{ fA/cm}^2$. These characteristics are shown to be stable at temperatures up to 350°C . The MIS(p^+) contacts fail to achieve equivalent results both in terms of thermal stability and contact characteristics but may still offer advantages over directly metallized contacts in terms of manufacturing simplicity. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4900539>]

I. INTRODUCTION

High-efficiency solar cells require low carrier recombination at their surfaces to ensure high open-circuit and maximum power point voltages. In recent years, focused research into the electronic passivation of $c\text{-Si}$ surfaces has resulted in the application of a wide range of high quality, industry applicable films for surface passivation, including SiO_2 , $\text{SiN}_x\text{:H}$, Al_2O_3 , $a\text{-Si:H}$, and stacks of these materials. As a consequence, the issue of surface recombination in the non-contacted surface regions of solar cells has diminished in importance, and recombination in the metallized regions has become one of major limiting factors of high efficiency homojunction solar cells.

In principle, the reduction of recombination at the contact interface can be achieved by the insertion of a thin dielectric interlayer between the silicon surface and the contacting metal, known as a metal-insulator-semiconductor (MIS) structure. The contact resistivity of MIS structures is strongly sensitive to both the thickness and the electronic properties of the dielectric, necessitating very precise control.¹ A simplified theoretical figure-of-merit for comparing MIS contacts with different insulator types and thicknesses is given by^{2,3}

$$f = d \sqrt{m_{(e,h)}^* \Phi_{\text{eff}(C,V)}}, \quad (1)$$

where d represents the insulator thickness, and $m_{(e,h)}^*$ and $\Phi_{\text{eff}(C,V)}$ are the tunneling effective mass of the collected carrier (electron or hole) and the effective barrier height presented to that carrier. A small value of the parameter f reflects a high tunneling probability, and hence a lower

contact resistivity. Also to be considered is the resistance presented by the dielectric layer to the other carrier, which should preferably be maximized. Hence, an ideal dielectric film would present a low barrier and effective mass to one carrier and a large barrier and effective mass to the other. Unfortunately, no such material has been demonstrated to have this attribute whilst simultaneously providing significant surface passivation. Resultantly, SiO_2 (Refs. 4–6) and Al_2O_3 (Refs. 7–9) have typically been used as the dielectric interlayers, as their thicker counterparts ($>100\text{ Å}$) have been successfully implemented for surface passivation in the non-contacted regions. However, given the wide band-gap of these dielectrics and the resultant large barrier heights they present to electrons and holes in $c\text{-Si}$, tunnel-able layers are limited to a maximum thickness of $\sim 25\text{ Å}$ in order to permit appreciable current flow. Achieving a high level of surface passivation with a 25 Å thick dielectric (or thinner) remains a difficult task, compromising the benefit of implementing this type of MIS contact.

It has been shown that capping of thin dielectrics ($\sim 10\text{ Å}$) with silicon-based hydrogen-rich films can lead to dramatic improvements in surface passivation.^{10,11} The enhancement is often attributed to the diffusion of atomic hydrogen from the capping film to the $c\text{-Si}$ /dielectric interface where it deactivates recombination centers. This suggests that plasma-enhanced-chemical-vapor-deposited (PECVD) hydrogenated amorphous silicon ($a\text{-Si:H}$), with its high hydrogen content (10%–20%)¹² could fulfill the requirements of a capping film.

A second interesting characteristic of $a\text{-Si:H}$ is its low-temperature interaction with metals, specifically with aluminum.¹³ At annealing temperatures well below the Al-Si eutectic temperature (577°C) silicon will dissolve into

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aluminum in low concentrations.¹⁴ The rate of dissolution is faster if the silicon is amorphous and faster still if the amorphous film has a high hydrogen concentration.¹⁵ Once dissolved, the silicon atoms can diffuse through the aluminum and crystallize out at nucleation points (defects, surfaces, grain boundaries, etc.), most likely with an aluminum doping concentration at the solubility limit.^{16,17}

This paper provides a proof-of-concept of a simple procedure for achieving well-passivated MIS-type contacts using the above mentioned two characteristics of *a*-Si:H. The complete contact structure consists of a lightly doped phosphorus (n^+) or boron (p^+) surface, followed by a tunneling dielectric layer, which is capped with intrinsic *a*-Si:H. Thin Al_2O_3 and SiO_2 layers are implemented as the tunneling dielectrics on p^+ and n^+ *c*-Si surfaces, respectively. These combinations are chosen in line with previous results of low surface recombination, assisted at least in part by the accumulation of majority carriers at the surface by the fixed charge density of the Al_2O_3 and SiO_2 films. As the additional intrinsic *a*-Si:H layer presents an impediment to current flow, following deposition is subsequently alloyed with an overlying aluminum film to create a high conductivity mixed-phase layer. The result is a contact structure that presents a contact resistivity ρ_c similar to that of conventional MIS contacts, together with a much lower recombination current J_{0c} , thanks to interface hydrogenation. Similar processes have previously been exploited for low temperature *pn* junction formation¹⁷ and low resistance metal-silicon contacts (contact formation to *a*-Si:H passivated wafers by means of annealing, “COSIMA”).¹⁸ It is also possible that the hydrogenation provided by the *a*-Si:H over layer could prove beneficial in the passivation of defects within the *c*-Si, for example, boron oxygen defects¹⁹ and laser damaged regions.²⁰

A crucial parameter in the success of the above described *a*-Si:H enhanced MIS contact is the annealing temperature—one must be chosen at which aluminum interacts with the *a*-Si:H but not with the underlying thin dielectric. For the Al/ SiO_2 system, the maximum temperature of stability has been estimated to be in the range of 200–400 °C,²¹ whilst it is expected that the Al/ Al_2O_3 interaction will initiate at lower temperatures.¹ Section III below presents an optimization of the annealing temperature, complemented with transmission/scanning transmission electron microscopy (TEM/STEM) and energy dispersive x-ray (EDX) spectroscopy analysis of changes to the layer composition. Once the fabrication process of the contact system is developed, the study proceeds to alter the thickness of the dielectric interlayer to find the best combination of contact characteristics.

The efficacy of the contact system, i.e., its selectivity towards electrons and holes, can be monitored by considering its resistive and carrier recombination properties. The contact resistivity ρ_c reflects the (undesired) resistance presented to the collected carrier (contact majority carrier), whereas the recombination current parameter of the contact J_{0c} provides information on the (desired) resistance or “blocking” action presented to the minority carrier. Whilst it is intuitive that simultaneous minimization of ρ_c and J_{0c} leads to improvements in contact-selectivity, understanding

the potential benefits of applying these contacts at the device level is not. Consideration must be made of the physical configuration, in which the contacts are to be applied. To address this point, Sec. IV includes device simulations to determine the optimum ρ_c – J_{0c} combination and corresponding contact configuration.

II. FABRICATION AND CHARACTERIZATION OF THE CONTACT STRUCTURES

To characterize the properties of the contacts, symmetrical test structures were prepared on float-zone, $>100 \text{ } \Omega\text{cm}$ resistivity, (100) oriented, p and n-type Si wafers. After saw damage etching and standard RCA cleaning, the wafers were diffused in quartz furnaces with boron (on n-type wafers) or phosphorus (on p-type wafers) so that in all cases the doping of the diffusion and substrate were opposed. A post diffusion alkaline etch was performed on the phosphorus diffusion to lower its surface concentration and increase the sheet resistance. Figure 1 provides the final dopant profiles of the boron (p^+) and phosphorus (n^+) diffusions as determined by electrochemical capacitance voltage measurements (WEP Wafer Profiler).

Following another RCA clean, p^+ samples were coated symmetrically at 200 °C with between 2 and 25 cycles of thermal atomic-layer-deposited (ALD) Al_2O_3 films (Beneq TFS 200). Alternating cycles of trimethylaluminum and water were used with pulse and purge durations chosen in line with a self-limiting reaction. The ALD growth rate, as measured from thicker films, was found to be $\sim 1 \text{ } \text{\AA}/\text{cycle}$; although for the ultra-thin films used in this study, the growth rate cannot be assumed to be perfectly linear.²²

SiO_2 films were grown into the n^+ samples in a clean quartz furnace at either 700 °C or 800 °C in pure oxygen (oxidation times typically less than 60 s), resulting in film thicknesses between 1.3 and 2.0 nm. Following the deposition/growth of dielectrics, the samples were symmetrically capped with PECVD *a*-Si:H. Interestingly, different

FIG. 1. Measured dopant profiles of p^+ and n^+ diffusions used in this study. The inset table provides details of the sheet resistance (R_{sh}) and surface dopant concentration (N_{surf}) as well as reference recombination factors representative of the metallized ($J_{0\text{metal}}$), passivated ($J_{0\text{pass}}$), and simulated ideal ($J_{0\text{ideal}}$) surfaces on the n^+ and p^+ diffusions.

optimum capping a -Si:H films (deposited by different PECVD tools) were found for the p^+ and n^+ samples. The p^+ samples were coated with ~ 30 nm of a -Si:H at a deposition temperature of $\sim 200^\circ\text{C}$ (Oxford PlasmaLab 100) and subsequently annealed for 15 min at 400°C in forming gas ambient to activate the passivation. The n^+ samples were coated with ~ 30 nm of a -Si:H at $\sim 300^\circ\text{C}$ (Roth & Rau AK400) and required no post-deposition anneal to activate the passivation. Aluminum was then evaporated symmetrically onto all samples to a thickness of ~ 10 nm to mimic the metal contacts whilst allowing sufficient light through, in order to use the photoconductance decay (PCD) method to measure the effective minority carrier lifetime. PCD measurements were taken using a Sinton WCT120 instrument, and contact recombination factors J_{0c} were extracted using the Kane and Swanson technique²³ with an intrinsic carrier concentration $n_i = 8.6 \times 10^9 \text{ cm}^{-3}$ (at 297 K).

Included in the inset of Figure 1 are reference values of the optimally passivated $J_{0\text{pass}}$, directly metallized $J_{0\text{metal}}$, and simulated ideal $J_{0\text{ideal}}$ recombination factors of the p^+ and n^+ dopant profiles used in this study. The $J_{0\text{pass}}$ represents the lowest recombination factor that has been achieved experimentally for the p^+ and n^+ dopant diffusions, and is representative of non-contacted regions with state-of-the-art surface passivation. The $J_{0\text{pass}}$ values were obtained in a separate study via PECVD a -Si:H (~ 30 nm) for the n^+ surface and ALD Al_2O_3 (~ 20 nm) for the p^+ surface, in-line with previously reported low surface recombination results on these doped surfaces.^{13,24} The metallized recombination parameters $J_{0\text{metal}}$ were measured on samples with ~ 10 nm of aluminum evaporated directly onto the diffused surfaces. These values are representative of the recombination factor in the contacted regions if metallization is applied directly to the c -Si. The ideal recombination factors $J_{0\text{ideal}}$ were simulated from the measured dopant profiles using Boltzmann statistics and the assumptions of no surface recombination (Auger recombination,²⁵ mobility,²⁶ and band gap narrowing^{27,28} models were utilized in this simulation).²⁹ These values represent the theoretical minimum recombination factors that can be achieved with the dopant profiles in Figure 1. It is worth noting that the measured $J_{0\text{pass}}$ recombination factors are, within measurement error, approximately equal to the simulated $J_{0\text{ideal}}$ values, indicating that surface recombination has been almost completely suppressed in the optimally passivated references.

Transfer-length-method (TLM) samples were fabricated on the same substrates, and using an identical procedure to the lifetime test samples up until the aluminum evaporation, which was instead deposited to a thickness of $\sim 1 \mu\text{m}$ on only one side. The TLM contact pad patterns were photolithographically defined and isolated using an acidic metal etch. Pad spacings of 10–300 μm were used in this study. Current–voltage measurements were performed at ~ 297 K (Keithley 2425 Source Meter) and ρ_c was extracted as per the description given in Ref. 30.

STEM samples were prepared on single-side polished silicon wafers. Thermal SiO_2/a -Si:H/Al contact structures were deposited on the polished surface, following which TEM lamellae were prepared by mechanical tripod polishing

and ion milling. An FEI Tecnai Osiris instrument was used to take bright field (BF) and high angle annular dark field (HAADF) STEM micrographs and high sensitivity EDX maps of local aluminum, silicon, and oxygen concentrations. Contact structures with an Al_2O_3 tunnel layer were not analyzed by STEM and EDX micrographs due to ambiguity in the aluminum EDX signal.

Film thicknesses were monitored by fitting polarized reflectance data (J.A. Woolam M2000 ellipsometer) of single side polished silicon wafers deposited alongside lifetime and TLM samples. Given the dependence of SiO_2 growth on dopant concentration, the SiO_2 thickness samples were subjected to a phosphorus diffusion prior to oxidation to create an alike surface concentration.

Implicit in this study is the assumption that lifetime samples (with ~ 10 nm of aluminum) and TLM samples ($\sim 1 \mu\text{m}$ of aluminum) behave identically in terms of contact recombination. To explore the validity of this assumption, photoluminescence (PL) images were taken (BT Imaging LIS-R1) of a symmetrically passivated c -Si(n^+)/ SiO_2 (1.6 nm)/ a -Si:H sample. On the rear side of this sample, half the area was covered with thick aluminum (1 μm) and the other half with thin aluminum (~ 10 nm). Figure 2 provides PL images of the sample taken with and without a 1000 nm short pass (SP) filter, after a 40 min, 250°C anneal step (see Sec. III A). Without the SP filter, greater rear-side reflection from the thick aluminum results in contrast between the two regions. With the filter, the effect of rear-side reflection is removed due to a penetration depth shallower than the thickness of the sample. An absence of contrast between the thick and thin aluminum regions in this image suggests that in both regions the carrier density profiles are very similar, and hence so are their respective surface recombination characteristics.

III. OPTIMIZATION OF THE ALUMINUM-AMORPHOUS SILICON INTERMIXING

A. Temperature dependence of the characteristic contact parameters

A significant component in the implementation of the proposed contact structure is the low-temperature interaction between a -Si:H and aluminum. To investigate the lowest temperature at which the Al/ a -Si:H interaction will commence, Al/ a -Si:H/ $\text{Al}_2\text{O}_3/c$ -Si(p^+) (referred to hereafter as

FIG. 2. PL images of an Al/ a -Si:H/ SiO_2 (~ 1.6 nm)/ c -Si(n^+) sample taken with and without a 1000 nm short-pass filter. The two images are scaled individually to enhance contrast.

MIS(p⁺) and Al/*a*-Si:H/SiO₂/*c*-Si(n⁺) (referred to hereafter as MIS(n⁺)) TLM structures were fabricated and annealed at different temperatures and ρ_c was monitored as a function of annealing time. Figure 3 shows the dependence of ρ_c on annealing time for the two contact structures, annealed at 200 °C and 250 °C. In this particular instance, the MIS(n⁺) and MIS(p⁺) structures had insulator thicknesses of ~ 1.6 nm. It should be noted that the ρ_c values $\geq 1 \Omega \text{ cm}^2$ were extracted from current-voltage measurements that deviated from pure Ohmic behavior and, as such, they represent a lower-limit ρ_c . As a reference, the directly metallized ρ_c values measured for the n⁺ and p⁺ surfaces are also provided in Figure 3. A slight reduction in ρ_c over the 40 min period is seen for the 200 °C anneal, however, the reduction in ρ_c is prohibitively slow. Instead, annealing at 250 °C provides an acceptable ρ_c for solar cell contacts after 20 min, for both the MIS(p⁺) and MIS(n⁺) contacts. Additional annealing reduces ρ_c only slightly, after which ρ_c appears to saturate to a value of $\sim 10 \text{ m}\Omega \text{ cm}^2$, which is still three orders of magnitude higher than for the directly metallized case. The saturation of ρ_c after 40 min of annealing suggests that the conductivity of the previously *a*-Si:H is layer is no longer the limiting factor of conduction, and that now the tunneling interlayer dominates the measured resistivity. As demonstrated in Section IV A, the final saturated ρ_c values are strongly dependent on the dielectric thickness, suggesting that further optimization is possible.

As shown in Sec. IV A below, the J_{0c} attainable with the *a*-Si:H enhanced MIS structures is significantly lower than that of basic MIS type contacts (without the *a*-Si:H capping) and that both structures show a strong J_{0c} dependence on the dielectric layer thickness. In the case of a ~ 1.6 nm film, as used in Figure 3, the J_{0c} prior to the alloying step were ~ 40 and 90 fA/cm^2 for the *a*-Si:H enhanced MIS(n⁺) and MIS(p⁺), respectively. Over the 40-min, 250 °C alloying anneal the J_{0c} of the MIS(n⁺) contact did not change significantly, remaining within the margins of measurement uncertainty. The J_{0c} of the MIS(p⁺) contact increased by approximately a factor of two under these conditions, from 90 to $\sim 160 \text{ fA/cm}^2$.

FIG. 3. Anneal time dependent ρ_c for MIS(p⁺) and MIS(n⁺) contacts with ~ 1.6 nm dielectric layers. Lines provide a guide to the eyes only and error bars are based on the estimated measurement error. Dotted horizontal lines represent directly metallized ρ_c values for the n⁺ and p⁺ diffusions.

The annealing conditions described above reflect the lowest temperature at which the *a*-Si:H/Al interaction, and hence contact formation, will occur. Some conventional solar cell processing steps, such as the application of PECVD *a*-SiN_x:H passivation and antireflection coating, require temperatures of up to 400 °C. Hence, it is of interest from a processing perspective to know the stability of J_{0c} at those temperatures as well. Provided in Figure 4 are the J_{0c} values for the MIS(p⁺) and MIS(n⁺) contacts as a function of anneal time for annealing temperatures between 300 °C and 400 °C. All samples received a 40 min, 250 °C anneal prior to the commencement of the higher temperature annealing. The J_{0c} of the MIS(n⁺) exhibits no significant increase after 45 min at 350 °C; however, at 400 °C the J_{0c} underwent a 10 fold increase over the same time period. This is in alignment with temperatures reported in the literature for the initiation of the SiO₂/Al interaction,²¹ suggesting that aluminum may be moving through the oxide layer.

The MIS(p⁺) exhibited a poorer stability at 350 °C, increasing to over $\sim 1000 \text{ fA/cm}^2$ —close to the directly metallized $J_{0\text{metal}}$ value of $\sim 1350 \text{ fA/cm}^2$ given in Fig. 1. Nevertheless, a reasonable stability was observed for the MIS(p⁺) at 300 °C, with a final J_{0c} of $\sim 500 \text{ fA/cm}^2$ after 45 min of annealing, a value well below the directly metallized case.

Contact resistance measurements taken after higher temperature annealing revealed small reductions in ρ_c but remained orders of magnitude above the directly metallized case—again supporting the conclusion that ρ_c is now dominated by tunneling through the dielectric layer.

B. Temperature dependent compositional analysis

To investigate the compositional changes responsible for the above discussed thermal dependence of the contact characteristics, STEM analysis and accompanying EDX mapping of local Al, Si, and O concentrations were performed on MIS(n⁺) contacts. As a baseline from which to compare annealed samples, an Al/*a*-Si:H (~ 30 nm)/SiO₂ (~ 2 nm)/*c*-Si contact structure was imaged before the alloying anneal. Figure 5(a) provides a HAADF STEM image and

FIG. 4. Temperature stability of MIS(p⁺) and MIS(n⁺) as assessed by changes in J_{0c} . Lines provide a guide to the eyes only, error bars are based on the estimated measurement error.

FIG. 5. HAADF STEM and EDX line scans of local Al, O, and Si distribution for (a) an Al/*a*-Si:H (~ 30 nm)/SiO₂ (~ 2 nm)/*c*-Si contact in its as-deposited state and (b) an Al/*a*-Si:H (~ 30 nm)/SiO₂ (~ 50 nm)/*c*-Si contact after 40 min alloying at 250 °C. The line-scans account for the differences in both composition and density of the different films.

corresponding EDX line-scans of the local Al, Si, and O distribution of the un-annealed contact. Evident in the HAADF STEM image are the SiO₂, *a*-Si:H and Al layers on *c*-Si, with an additional unintentional interlayer between the *a*-Si:H and SiO₂ layers. No evidence of significant interaction between the Al and *a*-Si:H layers is seen in the STEM image, as supported by the EDX line scans which show a sharp decline in Al accompanied by a sharp increase in Si concentration at the Al/*a*-Si:H interface. These line scans also suggest that the intermediate layer between the SiO₂ and *a*-Si:H layers is a sub-stoichiometric oxide species (SiO_{x<2}). Additional high-resolution (HR) TEM micrographs (not shown here) of the *a*-Si:H layer revealed no sign of crystallization.

To inspect the compositional changes at 250 °C, STEM imaging and EDX mapping and line scans of an Al/*a*-Si:H (~ 30 nm)/SiO₂ (~ 50 nm)/*c*-Si structure after a 40 min at 250 °C anneal were undertaken. A thicker SiO₂ layer was used in this instance to obtain a clearer distinction between interfaces. Figure 6(a) shows the HAADF STEM image and corresponding Al, Si, and O EDX mappings of the annealed contact structure. In contrast to the un-annealed sample, the Al mapping in Figure 6(a) shows a local protrusion of Al through the previously deposited *a*-Si:H layer, with an Al

accumulation at the SiO₂ surface. This is supported by a corresponding low Si concentration in the same region as seen in the Si EDX mapping. It appears that the SiO₂ layer limits any significant movement of Al further towards the *c*-Si at this annealing temperature. The EDX line scans included in Figure 5(b) illustrate the compositional variation through one of these local Al rich regions and show accumulation of Al at the SiO₂ surface. Localized atomic composition analysis reveals a small silicon concentration (~ 1 at. %) in the Al layer, indicating partial dissolution of Si into Al. More significantly, Al concentrations of up to 40 at. % are detected in the underlying *a*-Si:H film. These concentrations, which are well above the doping solubility limit, suggest that the previously *a*-Si:H layer is now semi-metallic and hence highly conductive. The saturation in ρ_c seen in Figure 3 is therefore likely dominated by carrier tunneling through the still intact thin dielectric layer. The region of high Al concentration within the *a*-Si:H layer is seen to be correlated with a region of contrast in the HAADF STEM image. HR TEM micrographs of the same region reveals lattice fringes indicative of the presence of crystallites, as shown in Figure 7.

Additional thermal treatment for 15 min at 400 °C results in aluminum completely replacing the previously *a*-Si:H layer, with a compositional concentration close to 100%, as seen in Figure 6(b), which shows the EDX mapping after this anneal step. Also evident in this figure is that the SiO₂ layer is acting as a barrier to further Al diffusion. The preservation of the SiO₂ layer is consistent with the results for MIS(n⁺) in Figure 4, which indicate that after 15 min at 400 °C the J_{oc} is ~ 250 fA/cm², still much lower than the corresponding value for the directly metallized surface. A HR TEM image, shown in Figure 7, reveals extensive crystallization (of aluminum-rich regions) in the previously *a*-Si:H layer.

IV. THE TRADE-OFF BETWEEN RECOMBINATION CURRENT AND CONTACT RESISTANCE

A. Dependence of contact characteristics on insulator thickness

Using the 40-min, 250 °C anneal identified in Sec. III A as optimal, the contact characteristics of MIS(n⁺) and MIS(p⁺) structures with differing insulator thicknesses were

FIG. 6. HAADF STEM and EDX mappings of the local Al, O, and Si concentrations for an Al/*a*-Si:H (~ 30 nm)/SiO₂ (~ 50 nm)/*c*-Si contact (a) after 40 min annealing at 250 °C and (b) after an additional 15 min annealing at 400 °C.

FIG. 7. HR TEM micrographs showing signs of crystallization in the a -Si:H layer for Al/ a -Si:H (~ 30 nm)/SiO₂ (~ 50 nm)/ c -Si contact structures annealed at 250 °C for 40 min (left) and at 250 °C for 40 min with an additional 15 min at 400 °C (right).

measured. As a baseline from which to compare these results, a set of reference MIS samples were also prepared on identical dopant diffusions, without the a -Si:H capping step (referred to hereafter as basic MIS). Figures 8(a) and 8(b) provide the ρ_c and J_{0c} dependence on SiO₂ thickness, for the a -Si:H capped MIS(n^+) contact, alongside the corresponding basic MIS(n^+) reference samples. Also included in these plots are horizontal dotted lines corresponding to the directly metallized ρ_c and $J_{0\text{metal}}$ and the optimally passivated $J_{0\text{pass}}$. In agreement with the theoretical probability for quantum-mechanical tunneling, a strong increase in ρ_c is observed as a result of increasing dielectric thickness—spanning more than three orders of magnitude for a 5 Å difference in SiO₂ thickness. Over the range measured, it can be seen that there is no significant difference in the thickness dependence of ρ_c between the a -Si:H capped and basic MIS structures. This further supports the conclusion that following the alloying step,

the passage of current through the a -Si:H capped MIS(n^+) is, like the basic MIS(n^+) structure, limited only by carrier tunneling through the dielectric layer.

Coupled with the increasing ρ_c as a function of dielectric thickness is a decreasing J_{0c} . The a -Si:H capped and basic MIS(n^+) structures both offer a significant reduction in recombination, as compared to the directly metallized case. In addition, it can be seen that for both structures, converse to the ρ_c trend, J_{0c} decreases with increasing insulator thickness. Most significantly, it can be seen that the J_{0c} of the a -Si:H capped MIS(n^+) is consistently almost an order of magnitude lower than the basic MIS(n^+). A dielectric thickness of 1.7 nm is sufficient to achieve the lower limit (optimally passivated) recombination factor of ~ 25 fA/cm², but at the expense of a high ρ_c . This value is approximately identical to that corresponding to Auger recombination within the n^+ region, which suggests that even lower recombination factors may be attainable by reducing the dopant dose of the underlying diffusion. The 700 and 800 °C oxides exhibit similar ρ_c and J_{0c} trends; a slightly earlier transition to lower J_{0c} and higher ρ_c for the higher temperature oxide may reflect differences in the density of the two SiO₂ films.

An analogous set of results for the MIS(p^+) contact characteristics as a function of the number of ALD Al₂O₃ cycles is provided in Figures 8(c) and 8(d). Similar to the trend seen for the MIS(n^+) structures, both the a -Si:H capped and basic MIS(p^+) structures exhibit alike contact resistance dependences on thickness. Structures which were fabricated with more than 15 ALD cycles (~ 1.5 nm) were measured to produce large ρ_c values and general nonlinear current-voltage behavior. The rapid onset of high resistance contact behavior seen for both MIS(p^+) structures is attributable to the large valence band offset between the c -Si and Al₂O₃ (Ref. 31) and the corresponding high value of f (Eq. (1)).

In terms of recombination, again both the a -Si:H capped and basic MIS(p^+) structures produce lower recombination factors than the directly metallized case, with the a -Si:H capped structures producing the lowest recombination

FIG. 8. Contact resistivity ρ_c of (a) MIS(n^+) and (c) MIS(p^+) structures and contact recombination factor J_{0c} for (b) MIS(n^+) and (d) MIS(p^+) structures as a function of insulator thickness. Lines provide a guide to the eyes only, error bars are based on the estimated error in measurement. The adjacent plot includes some data which have previously been presented elsewhere.³⁵

FIG. 9. Simulated optimum contact fraction m_f (dashed lines) and resultant idealized efficiency (contour plot) as a function of rear contact ρ_c and J_{0c} for (a) n^+ contacts and (b) p^+ contacts presented in this paper. All values to the right of the 100% contact fraction lines were simulated with full area contacts. Directly metallized, basic MIS, and a -Si:H capped MIS data points are superimposed on top of the contours to reflect their relative carrier-selectivity. The varied parameter in the MIS contact data trends is the insulator layer thicknesses.

factors within the dielectric thickness range of relevance. However, the level of passivation is consistently less than that provided by the MIS(n^+) structures—reaching at best ~ 150 fA/cm²—which is significantly higher than the optimally passivated case, but still approximately an order of magnitude lower than the directly metallized p^+ surface. The passivation quality of the a -Si:H enhanced MIS(p^+) appears to stop improving after ten cycles of Al₂O₃—producing a local minimum.

The lower level of surface passivation could be associated with a minority/majority capture cross-section ratio σ_n/σ_p greater than unity, which is expected for the recombination active defects present at the Al₂O₃/c-Si interface.³² In addition, the relatively low work function of aluminum may induce downwards band bending increasing the minority carrier concentration at the c-Si surface. A metal with a higher work function which also interacts with a -Si:H at low temperatures may prove to be more appropriate for the MIS(p^+), for example, nickel³³ or gold.³⁴

B. Significance to solar cells

The trends presented in Sec. IV A are revealing in themselves, showing the diverging behavior of contact passivation and conductivity with the dielectric layer thickness. This opposing behavior highlights the difficulty in determining the best ρ_c - J_{0c} combination. The simplest application of the contact structures described in this paper would be as a full area

contact on the rear side of solar cells. But, as it is well known, it is also possible to form the contact only in part of the rear surface, either as dots or lines. In a device design with partial rear contacts, the remaining surfaces can be passivated by an appropriate dielectric film. This design implies that carrier flow towards the contacts is geometrically constricted,^{36,37} thus adding an element of resistance, for both majority and minority carriers, to the specific contact characteristics ρ_c and J_{0c} . Therefore, to properly evaluate a given contact system, it is necessary to consider the geometric configuration in which the contact is to be applied. The latter is globally represented by the fraction of the rear surface occupied by the contact m_f .

To compare contact structures, we have modelled an idealized solar cell structure with partial rear contacts using the freeware solar cell simulation program Quokka2.³⁸ In these simulations, losses due to front surface recombination, resistance, and shading have been reduced to a minimum or removed completely in order to emphasize the influence of the rear contact. The rear contact is simulated with a variable ρ_c and J_{0c} ; for every ρ_c - J_{0c} combination an optimum contact fraction m_f is calculated (dashed lines)—and from this configuration an idealized efficiency is obtained (contours). These results are presented in Figures 9(a) and 9(b) for the contacts on n^+ and p^+ diffusions, respectively. Assumptions used in the simulations are detailed in Table I. Both simulations show almost identical results, this is attributable to the very similar resistivity and recombination characteristics of the n^+ and p^+ diffusions used in this study.

TABLE I. Parameters, assumptions, and structure used in the idealized cell simulations.

Symbol	Parameter	Assumption/value	Simulation structure
$J_{0\text{front}}$	Front recombination factor	1 fA/cm ²	
τ_{bulk}	Bulk lifetime	Richter <i>et al.</i> intrinsic lifetime ²⁵	
J_g	Generation current density	~ 42 mA/cm ²	
W	Wafer thickness	160 μm	
ρ_{bulk}	Bulk type, resistivity	1 Ω cm n-type (Fig. 9(a)) 1 Ω cm p-type (Fig. 9(b))	
$J_{0\text{rear}}$	Rear recombination factor (in non-contacted area)	$J_{0\text{ideal}}(p^+) = 23.4$ fA/cm ² (Fig. 9(b)) $J_{0\text{ideal}}(n^+) = 24.8$ fA/cm ² (Fig. 9(a))	
$R_{\text{sh_rear}}$	Rear diffusion sheet resistance	100 $\Omega/\square$	
m_{rear}	Rear line-contact metal fraction	Finger width = variable Finger pitch = 1000 μm	

By superimposing the experimentally measured thickness dependent ρ_c - J_{oc} trends (presented in Figure 8) on these plots, the insulator thickness which provides the optimum ρ_c - J_{oc} configuration is identified as the point which falls within the region of highest efficiency. It can be seen that the trends in efficiency are parallel with the concept of carrier-selectivity described in the introduction. That is, reductions in the majority carrier resistivity and minority carrier recombination lead to improvements in carrier-selectivity and hence efficiency.

Similarly, the trends in optimum m_f provide information on the ease of fabrication for a particular contact, with larger m_f values being easier to fabricate. It is worth mentioning that no technological constraints are placed on the width of the rear fingers used in these simulations. Hence, real-world realization of contacts with simulated small optimum m_f values would likely be constrained technologically to larger fractions with lower corresponding efficiencies than those seen in Figure 9.

Included in Figure 9(a) are data points which reflect the contact characteristics of the directly metallized n^+ contact MS(n^+), the basic MIS(n^+) and the a -Si:H capped MIS(n^+). This comparison reveals that in this particular instance, the only benefit gained in using the basic MIS(n^+) over the directly metallized MS(n^+) contact is the ability to use larger contact fractions at the expense of relatively modest decreases in device efficiency. Integrating the a -Si:H capping step, however, is shown to improve the carrier-selectivity (hence efficiency) whilst simultaneously increasing the optimum m_f value. The highest idealized efficiencies of $\sim 26.1\%$ are obtained on a -Si:H capped MIS(n^+) structures with a ~ 1.55 nm SiO_2 film which produce a ρ_c - J_{oc} combination of ~ 3 m Ω cm 2 and ~ 40 fA/cm 2 . These values are simulated with an optimum m_f value between 30% and 50%—a fraction easily achievable using today's industrial processes.

An alike evaluation of the p^+ contacts presented in Figure 9(b) reveals a significant loss in carrier-selectivity as a result of transitioning from the directly metallized MS(p^+) to the basic MIS(p^+). This is due primarily to a larger ρ_c . The a -Si:H capped MIS(p^+) also shows small losses in efficiency over the directly metalized case when both are applied in their optimum m_f , with corresponding optimized efficiencies of $\sim 25.9\%$ and $\sim 26.0\%$, respectively. It can be summarized that the only benefits associated with using either MIS(p^+) contacts is that the lower recombination factors allow the contact to be applied in a larger fraction. The MIS results on p^+ surfaces might be improved by choosing an alternative to Al_2O_3 with a lower figure of merit f (Eq. (1)) and a metal with a larger work function.

V. CONCLUSION

A fabrication procedure for carrier-selective MIS contacts that utilizes an a -Si:H capped dielectric tunneling layer has been presented. Lightly diffused (~ 100 $\Omega/\square$) MIS(p^+) and MIS(n^+) structures, employing Al_2O_3 and SiO_2 dielectric layers, respectively, have been shown to greatly reduce recombination, while still permitting majority carrier transport. STEM and EDX analysis reveal that the alloying

between the a -Si:H capping layer and the Al over-layer is a crucial mechanism in the successful formation of the contact structure.

Based on solar cell device simulations, SiO_2 thicknesses in the range of 1.5–1.65 nm are found to be optimum for the MIS(n^+) contacts, resulting in ρ_c - J_{oc} combinations of ~ 3 m Ω cm 2 and ~ 40 fA/cm 2 . These simulations suggest that the MIS(n^+) contacts can be applied in large area fractions, and hence also offer advantages over established high efficiency silicon solar cell approaches in terms of process simplicity. The thermal stability of the MIS(n^+) contacts at 350 °C has also been demonstrated, suggesting that they can be integrated with a standard PECVD a -SiN $_x$:H process.

The MIS(p^+) contacts revealed poorer characteristics than MIS(n^+) contacts both in terms of thermal stability and ρ_c - J_{oc} combinations, but still offer advantages over conventional approaches based on selective dopant diffusions.

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