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## Amorphous silicon passivated contacts for diffused junction silicon solar cells

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Carrier recombination at the metal contacts is a major obstacle in the development of high-performance crystalline silicon homojunction solar cells. To address this issue, we insert thin intrinsic hydrogenated amorphous silicon [*a*-Si:H(*i*)] passivating films between the dopant-diffused silicon surface and aluminum contacts. We find that with increasing *a*-Si:H(*i*) interlayer thickness (from 0 to 16 nm) the recombination loss at metal-contacted phosphorus ( $n^+$ ) and boron ( $p^+$ ) diffused surfaces decreases by factors of  $\sim 25$  and  $\sim 10$ , respectively. Conversely, the contact resistivity increases in both cases before saturating to still acceptable values of  $\sim 50 \text{ m}\Omega \text{ cm}^2$  for  $n^+$  and  $\sim 100 \text{ m}\Omega \text{ cm}^2$  for  $p^+$  surfaces. Carrier transport towards the contacts likely occurs by a combination of carrier tunneling and aluminum spiking through the *a*-Si:H(*i*) layer, as supported by scanning transmission electron microscopy–energy dispersive x-ray maps. We explain the superior contact selectivity obtained on  $n^+$  surfaces by more favorable band offsets and capture cross section ratios of recombination centers at the *c*-Si/*a*-Si:H(*i*) interface. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4872262>]

### I. INTRODUCTION

High-efficiency homojunction silicon solar cells have reached a point in their development where carrier recombination at the metal-silicon contact has a significant and sometimes limiting effect on device performance. This is commonly evidenced by relatively low open-circuit voltage values, compared to, e.g., silicon-heterojunction (SHJ) solar cells, which do not apply metal directly to the crystalline silicon absorber.<sup>1</sup> This issue has spawned much research in the area of “contact passivation”.<sup>2–6</sup>

On homojunction solar cells, contact passivation can be achieved by inserting a thin dielectric interlayer that physically displaces the metal from the crystalline silicon (*c*-Si) surface, in a metal–insulator–semiconductor (MIS) type configuration. This was initially applied at the device level using thermally grown SiO<sub>2</sub><sup>2</sup> and has more recently been trialed with atomic-layer-deposited Al<sub>2</sub>O<sub>3</sub>.<sup>3</sup> A modification of this approach is to replace the metal with heavily doped poly-silicon, or another conductive over-layer, which further improves the selectivity of the contact.<sup>4,5</sup> The efficacy of the MIS type contact scheme is reliant on film-thickness control at the monolayer-level, as a delicate trade-off between increasing contact resistance and decreasing interface recombination exists for both SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub>.<sup>6</sup> This is directly linked to the wide bandgap of the dielectrics trialed so far and presents a significant challenge for industrial implementation.

In this article, we propose the use of intrinsic hydrogenated amorphous silicon (*a*-Si:H(*i*)) as an alternative interlayer. This film has a lower bandgap than the previously mentioned dielectrics and hence may offer a weaker dependence of the

contact resistivity on thickness. In addition, such films have silicon surface passivation properties on par with the best dielectrics. Both properties are already successfully exploited in the intrinsic buffer layers used in SHJ solar cells, yielding conversion efficiencies as high as 24.7%, to date.<sup>7</sup> As with most device structures containing *a*-Si:H(*i*), a strong restriction on the temperature of processing is required, as annealing may irreversibly deteriorate the microstructure and passivation properties of the films. The presence of doped over-layers and metals may place even greater restrictions on the thermal processing of the device. Doped over-layers can lower the defect-creation energy,<sup>8</sup> while many metals induce crystallisation and protrude through *a*-Si:H(*i*) at low temperatures.<sup>9</sup> In particular, the application of aluminum directly to *a*-Si:H(*i*), as is the case in this study, remains a contentious combination in the context of solar cells.<sup>9–11</sup>

The applicability of the *a*-Si:H(*i*) contact interlayer is trialed here on both boron ( $p^+$ ) and phosphorus ( $n^+$ ) diffused surfaces, usually employed as the hole and electron collecting regions in traditional silicon solar cells. A simplified representation of the equilibrium energy band diagram of the structures tested in this study is provided in Figure 1. Identical *a*-Si:H(*i*)/Al stacks are used for the boron and phosphorus contacts. The contact resistivity  $\rho_c$  and the recombination parameter of the metal-contacted dopant diffusions  $J_{0c}$  are taken as the two metrics of importance, where low values are desired for both. The results are examined in terms of increasing *a*-Si:H(*i*) interlayer thickness in an effort to find an optimum value. Scanning transmission electron microscopy (STEM) is used in conjunction with energy dispersive x-ray (EDX) mapping to investigate the nature of the interfaces and the conduction mechanisms.

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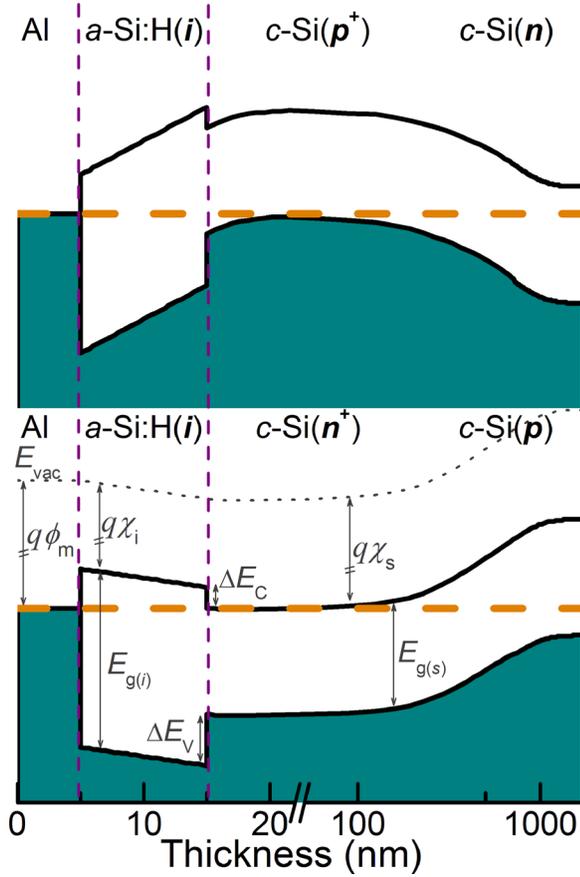


FIG. 1. Simplified equilibrium energy band diagrams representative of the hole-selective (top figure) and electron-selective (bottom figure) structures investigated in this study, as simulated by Automat for Simulation of Heterostructures (AFORS-HET).<sup>12</sup> Assumed values; Al work function  $\phi_m$  (4.23 V), *a*-Si:H(*i*) electron affinity  $\chi_i$  (3.8 V), *c*-Si electron affinity  $\chi_s$  (4.05 V), *a*-Si:H(*i*) mobility band gap  $E_{g(i)}$  (1.82 eV),<sup>13</sup> *c*-Si band gap  $E_{g(s)}$  (1.12 eV), *a*-Si:H(*i*)/*c*-Si valence band offset  $\Delta E_V$  (0.45 eV), and *a*-Si:H(*i*)/*c*-Si conduction band offset  $\Delta E_C$  (0.25 eV).<sup>13</sup>

## II. EXPERIMENTAL METHODS

### A. Sample preparation

Symmetrical test structures were prepared using high resistivity ( $>100 \Omega \text{ cm}$ ), (100), “Float-zone”, p and n-type silicon wafers. The high resistivity of these wafers simplifies the extraction of recombination parameters. They were subjected to a 2 min alkaline saw damage etch and their surfaces were chemically polished in a HF:HNO<sub>3</sub> solution. Following a standard RCA clean, the samples were diffused symmetrically in dedicated clean quartz furnaces using a POCl<sub>3</sub> source (on p-type wafers) or a BBr<sub>3</sub> source (on n-type wafers) so that in all cases the doping of the substrate and diffusion were of opposite polarity. Two diffusion recipes were used for each source; the phosphorus diffused samples underwent a further short etch-back process to reduce the surface dopant concentration. The resultant final attributes of the four diffusion sets are given in Table I.

Following another RCA clean, each of the diffusion sets was deposited symmetrically with thicknesses of *a*-Si:H(*i*), in the range of 1–16 nm, using an Oxford PlasmaLab 100 plasma-enhanced-chemical-vapor-deposition (PECVD) instrument. The wafer temperature during deposition was

TABLE I. Dopant diffusion characteristics and recombination parameters of the four diffusion sets.  $R_{sh}$ , sheet resistance;  $N_{surf}$ , surface concentration;  $J_{0\_metal}$ , recombination parameter of metallised diffusion region;  $J_{0\_pass}$ , recombination parameter of passivated diffusion region.

| Source            | $R_{sh}$ ( $\Omega/\square$ ) | $N_{surf}$ ( $\text{cm}^{-3}$ ) | $J_{0\_metal}$ ( $\text{fA}/\text{cm}^2$ ) | $J_{0\_pass}$ ( $\text{fA}/\text{cm}^2$ ) |
|-------------------|-------------------------------|---------------------------------|--|---|
| POCl <sub>3</sub> | 85 ± 5                        | 4(±1) × 10 <sup>19</sup>        | 1050 ± 200                                 | 55 ± 5                                    |
| POCl <sub>3</sub> | 110 ± 10                      | 3(±1) × 10 <sup>19</sup>        | 1200 ± 200                                 | 41 ± 5                                    |
| BBr <sub>3</sub>  | 110 ± 10                      | 1(±1) × 10 <sup>19</sup>        | 1370 ± 200                                 | 27 ± 5                                    |
| BBr <sub>3</sub>  | 170 ± 15                      | 1(±1) × 10 <sup>19</sup>        | 1900 ± 200                                 | 15 ± 5                                    |

estimated to be  $\sim 350^\circ\text{C}$ , which is uncharacteristically high for *a*-Si:H(*i*). At this temperature epitaxial growth of silicon is expected leading to poor quality surface passivation.<sup>14</sup> Despite this, we found this temperature to provide optimum passivation in the as-deposited state, suggesting that no epitaxial growth has occurred. At this point samples were further separated into two groups to be developed into symmetrical lifetime structures (for assessing the contact recombination) or transfer-length-method (TLM) structures (for assessing the contact resistivity).

The lifetime test structures were coated with aluminum on both sides in a vacuum thermal deposition system to a thickness of  $<15 \text{ nm}$ , which is sufficiently thin to allow light through for photoconductance decay (PCD) measurements to be taken. PCD measurements were performed using a Sinton WCT 120 instrument under both transient and quasi-steady-state modes. The recombination current parameters  $J_{0c}$  of the *c*-Si(*n*<sup>+</sup>)/*a*-Si:H(*i*)/Al and *c*-Si(*p*<sup>+</sup>)/*a*-Si:H(*i*)/Al stacks were extracted from the PCD data using an intrinsic carrier concentration of  $n_i = 8.95 \times 10^9 \text{ cm}^{-3}$  (at 25 °C) and the well-known Kane and Swanson method.<sup>15</sup> The parameter  $J_{0c}$  is a representation of the total minority carrier recombination occurring in the sub-surface diffusion region (predominantly Auger recombination) and at the diffused surface (predominantly Shockley–Read–Hall recombination).

TLM structures were created by evaporating  $\sim 1 \mu\text{m}$  of aluminum onto the *a*-Si:H(*i*) passivated *p*<sup>+</sup> and *n*<sup>+</sup> surfaces. Contact pads were photolithographically defined and isolated using an acidic aluminum etch. A 15 min 110 °C anneal is required to hard-bake the photoresist before the acidic etching. Current–voltage measurements were performed (Keithley 2425 Source Meter) at  $\sim 297 \text{ K}$  on pad spacings in the range of 10–300  $\mu\text{m}$  and  $\rho_c$  was extracted as per the description given in Ref. 16. As a point of clarification, in this study, the measured  $\rho_c$  reflects the average of both bias directions (implicit in TLM), where the resistivity in each direction comprises the resistance through the *a*-Si:H(*i*) as well as across the *a*-Si:H(*i*)/Al and *c*-Si/*a*-Si:H(*i*) interfaces. It was also assumed that the parallel sheet conductance between pads through the *a*-Si:H(*i*) layer is negligible.

### B. Reference recombination parameters

Included in Table I as a reference are the measured recombination parameters for diffusions covered by either only a metal film ( $J_{0\_metal}$ ) or a high-quality passivation film without a metal over-layer ( $J_{0\_pass}$ ). A thin aluminum layer ( $<15 \text{ nm}$ ) is used to create the directly metallized surface.

The high-quality passivation films consisted of  $\sim 20$  nm of plasma-assisted atomic-layer-deposited (PA-ALD)  $\text{Al}_2\text{O}_3$  (Beneq TFS, 200 ALD instrument) on the boron-diffused surfaces and  $\sim 75$  nm of PECVD  $a\text{-SiN}_x\text{:H}$  (Roth & Rau AK 400) on the phosphorus surfaces. The large positive fixed charge density in  $a\text{-SiN}_x\text{:H}$  and negative fixed-charge density in  $\text{Al}_2\text{O}_3$  reduce the minority carrier concentrations at the  $n^+$  and  $p^+$   $c\text{-Si}$  surfaces, respectively, which results in very low surface recombination even for moderate interface state densities. In comparison,  $a\text{-Si:H}(i)$  films exhibit no strong fixed charge, but achieve a very effective reduction of the density of interface states ( $<10^9 \text{ cm}^{-3}$ ),<sup>17</sup> making them ideal candidates for the passivation of both  $n^+$  and  $p^+$  surfaces.

Given the high quality of passivation obtained by the  $\text{Al}_2\text{O}_3$  and  $a\text{-SiN}_x\text{:H}$  layers, the  $J_{0\_pass}$  values provided in Table I can be viewed as an approximate upper-limit for the recombination occurring in the subsurface diffused regions, which is mostly due to the Auger process.

### C. Photoluminescence analysis

Inherent in the analysis to follow is the assumption that lifetime test structures (aluminum thickness  $<15$  nm) produce the same carrier recombination as actual (passivated) metal contacts, such as those present in the TLM test structures (aluminum thickness of  $\sim 1 \mu\text{m}$ ). To verify this assumption, a photoluminescence (PL) analysis (BT Imaging LIS-R1) was performed on two symmetrically diffused ( $n^+$ ) and passivated samples with  $\sim 15$  and  $\sim 30$  nm of  $a\text{-Si:H}(i)$ . On the rear side of the two samples, half of the area was evaporated with thin ( $<15$  nm) and the other half with thick ( $1 \mu\text{m}$ ) aluminum. Both samples were annealed at  $110^\circ\text{C}$  for 15 min before imaging. PL images were taken (rear side down) using a set illumination intensity with and without a short-pass filter of 1000 nm. The images taken without the filter are representative of a broader wavelength range and include longer wavelengths, which have a penetration depth greater than the thickness of the wafer. It is therefore expected that the region with the thicker aluminum (greater rear side reflection) will appear brighter, provided differences in carrier recombination are not significant. The image taken with the filter in place includes only wavelengths with penetration lengths significantly less than the thickness of the wafer—hence if there are no differences in carrier recombination, there should be no visible difference between the thick and thin metal regions. Figure 2 shows the two sets of PL images taken of the same region with and without a short-pass filter, where brighter colours represent a higher PL signal and thus longer effective carrier lifetime. In all cases, the above behavior is followed, demonstrating that there are no major differences in carrier recombination between the thin and thick metallisation schemes.

### D. Ellipsometry and transmission electron microscopy measurements

During all  $a\text{-Si:H}(i)$  depositions, a single side, mechanically polished wafer was included to monitor film thickness. Reflectance spectra of these samples were measured using a

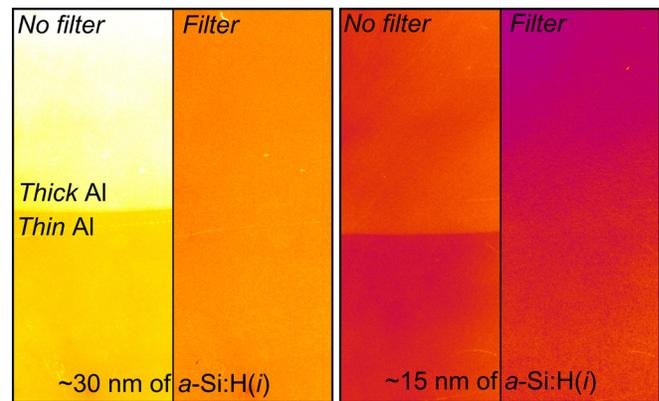


FIG. 2. PL images of samples with  $\sim 30$  and  $\sim 15$  nm of  $a\text{-Si:H}(i)$  taken with and without a short-pass filter. Without a filter images reveal different rear reflection. With a filter, the influence of rear reflection is removed, and the images indicate similar surface recombination for the two thicknesses of aluminum. All four images are scaled individually to highlight contrasts across the imaged region.

J.A Woolam M-2000 variable angle ellipsometer and thicknesses were obtained using a Tauc-Lorentz material model.<sup>18</sup>

STEM samples were also prepared from single-side mechanically polished wafers. These were deposited with  $\sim 28$  nm of  $a\text{-Si:H}(i)$  and  $\sim 1 \mu\text{m}$  of aluminum following which they were annealed at  $110^\circ\text{C}$  for 15 min. TEM lamellae were prepared by mechanical polishing in a wedge-shape configuration with a Tripod polisher then ion milling with Ar ions (Gatan PIPS). The preparation sequence before imaging required a temperature step at  $\sim 130^\circ\text{C}$  for over 30 min. An FEI Tecnai Osiris instrument was used to take bright field (BF) STEM micrographs and high sensitivity EDX maps of aluminum, silicon and oxygen.

## III. RESULTS AND DISCUSSION

### A. Interface passivation

The recombination current parameter  $J_{0c}$  as a function of  $a\text{-Si:H}(i)$  thickness is shown for the two phosphorus diffusions in Figure 3(a) and for the two boron diffusions in Figure 3(b). The quality of the as-deposited surface passivation on the phosphorus diffusion improves dramatically with  $a\text{-Si:H}(i)$  thickness and appears to saturate in the 6–8 nm range, consistent with open circuit voltage  $V_{oc}$  trends for SHJ solar cells reported in the literature.<sup>19</sup> Beyond these thicknesses excellent passivation is achieved, producing recombination parameters even lower (by about  $10 \text{ fA/cm}^2$ ) than the PECVD  $a\text{-SiN}_x\text{:H}$  controls listed in Table I, inferring that this value is a more appropriate upper-limit representation of recombination within the bulk of the phosphorus diffusion. An alike sample (not shown) deposited with  $\sim 30$  nm of  $a\text{-Si:H}(i)$  produces an identical  $J_{0c}$  to that at 10 nm confirming that the passivation is saturated. Whilst an expected slight difference in the magnitude of recombination between the 85 and 110  $\Omega/\square$   $n^+$  diffusions is seen, the general behaviour of both  $n^+$  diffusions can be well represented by a single trendline, adding to the confidence in the measured results.

Following metallisation, a significant increase in  $J_{0c}$  was observed for  $a\text{-Si:H}(i)$  thicknesses below 10 nm. The spread

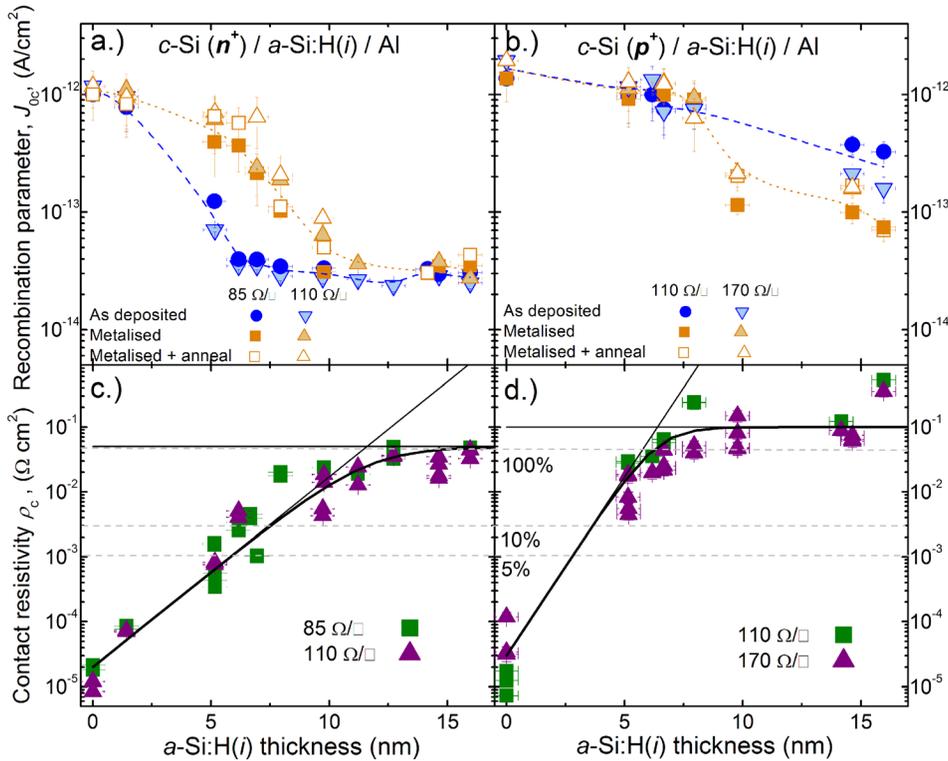


FIG. 3. Contact recombination parameter  $J_{0c}$  for (a) phosphorus and (b) boron diffused surfaces and contact resistivity  $\rho_c$  for (c) phosphorus and (d) boron diffused surfaces as a function of  $a\text{-Si:H}(i)$  thickness. The dotted blue and orange lines provide a guide to the eye for the as-deposited (blue) and metallised (orange) results. The dashed lines represent reference values for contacts with a total contact resistance  $R_c$  of  $\sim 0.05 \Omega\text{ cm}^2$ , having areas of respectively 5, 10, and 100% of the wafer surface (see Sec. III E). Error bars are based on the measured spread in data or the estimated error of the measurement (whichever was largest).

in measured data and uncertainty in determining  $J_{0c}$  values also greatly increase in this region, as indicated by the large error bars in Figure 3. Whilst there were some small increases in recombination evident for samples with  $a\text{-Si:H}(i)$  thicknesses above 10 nm, the  $J_{0c}$  values remained close to the corresponding pre-metallisation values. To provide a direct comparison to the TLM structures some of the metallised  $n^+$  symmetrical lifetime samples were annealed for 15 min at 110 °C as shown in Figure 3(a). It can be seen that whilst some additional increase in recombination is caused by the anneal, excellent passivation is still achievable for  $a\text{-Si:H}(i)$  thicknesses above 10 nm.

There are four foreseeable causes for the increase in  $J_{0c}$  when a metal overlayer is present: (i) penetration of the  $c\text{-Si}$  minority carrier wavefunctions through the  $a\text{-Si:H}(i)$  film to the  $a\text{-Si:H}(i)/\text{Al}$  interface, where rapid recombination is possible;<sup>20</sup> (ii) the onset of depletion conditions at the heavily diffused  $c\text{-Si}$  surfaces again caused by the aluminum work function, resulting in a change the recombination statistics at the  $c\text{-Si}$  surface;<sup>21,22</sup> (iii) a lowering of the Fermi-level within the  $a\text{-Si:H}(i)$  film by the aluminum work function, potentially leading to a lower defect formation enthalpy in the  $a\text{-Si:H}(i)$  film;<sup>8</sup> or (iv) partial protrusion of the aluminum through the  $a\text{-Si:H}(i)$ , possibly making contact with the  $c\text{-Si}$  surface.<sup>9</sup> A low temperature interaction between aluminum and  $a\text{-Si:H}(i)$  has been outlined in many previous studies,<sup>9–11</sup> some of which suggest that conditions experienced during aluminum vacuum depositions are sufficient to initiate this interaction. Below we confirm that indeed some aluminum spiking has occurred.

The boron diffused samples in Figure 3(b) show a more gradual improvement in as-deposited passivation with  $a\text{-Si:H}(i)$  thickness and do not achieve as good a level of passivation as the controls listed in Table I. Under these deposition conditions, an additional sample (not shown) with an

$a\text{-Si:H}(i)$  thickness of  $\sim 30$  nm produced a recombination parameter of  $\sim 70$  fA/cm<sup>2</sup> for both  $p^+$  diffusions, considerably lower than the 15 nm samples but still well above the controls listed in Table I. Avoiding a postdeposition anneal was a central premise of this work; hence, the deposition conditions were chosen to provide the highest as-deposited  $a\text{-Si:H}(i)$  passivation. However, in a separate study, we have found that the passivation provided by thicker  $a\text{-Si:H}(i)$  films ( $>12$  nm) improved upon annealing, presumably due to a reduction in  $D_{it}$  from additional hydrogenation. Therefore, lower  $J_{0c}$  may be attainable if a re-optimisation of the  $a\text{-Si:H}(i)$  films based on annealing was performed. Following metallisation,  $J_{0c}$  improved for  $a\text{-Si:H}(i)$  thicknesses greater than 10 nm, possibly due to a small annealing effect during the thermal evaporation of aluminum. Further annealing at 110 °C for 15 min resulted in no further improvement, rather in increases in  $J_{0c}$ . The higher surface recombination evident on the  $p^+$  surface relative to the  $n^+$  is potentially due to  $c\text{-Si}/a\text{-Si:H}(i)$  interface defects exhibiting an electron to hole capture cross section area ratio ( $\sigma_n/\sigma_p$ ) greater than unity.<sup>23</sup>

## B. Contact resistivity

The specific contact resistivity  $\rho_c$  for the phosphorus and boron diffusions as a function of  $a\text{-Si:H}(i)$  thickness are provided in Figures 3(c) and 3(d), respectively. For the phosphorus diffusion, the dependence of  $\rho_c$  on the thickness of the  $a\text{-Si:H}(i)$  interlayer can be separated into two regimes; an approximately exponential increase for the first 10 nm followed by a plateauing of  $\rho_c$ . This behavior appears to be largely independent of the underlying doping, as both the 85 and 100  $\Omega/\square$  diffusions yield similar trends.

Both boron-diffused surfaces exhibit a steeper initial increase in  $\rho_c$  and plateau at a higher value relative to the  $n^+$

surfaces. A potential explanation for the higher  $\rho_c$  on  $p^+$  surfaces may be found in the well-known asymmetry between the conduction and valence band offsets at the  $c$ -Si/ $a$ -Si:H( $i$ ) interface.<sup>13</sup> These offsets contribute to effective barriers for electron and hole transport at the  $c$ -Si surface, as depicted in Figure 1. A significantly smaller conduction band offset, as compared to the valence band offset has been reported by many studies at this interface which suggest a greater conductivity across the interface for electrons (in  $n^+$  silicon) than holes (in  $p^+$ ).<sup>13</sup> Studies of window layers in SHJ solar cells equally pointed out that the valence-band offset may hinder efficient hole transport through passivation stacks.<sup>24</sup> An additional possible explanation is the formation of a large energy barrier at the  $p^+$   $c$ -Si surface caused by the low work function of aluminum.<sup>21</sup> An alike barrier forming on the  $n^+$  surface would be smaller owing to a higher  $c$ -Si surface concentration (compared to the  $p^+$  contact) and a smaller difference between the  $n^+$   $c$ -Si Fermi energy and the Al work function.

### C. Structural composition of the layers

STEM-EDX analysis of the contact stack, presented in Figure 4, was taken to better understand the interfacial uniformity and conduction mechanisms. Figure 4(a) shows the bright field STEM image of a  $c$ -Si/ $a$ -Si:H( $i$ )/Al ( $1\ \mu\text{m}$ ) structure. Note that the  $a$ -Si:H( $i$ ) film was made intentionally thicker ( $\sim 28\ \text{nm}$ ) than the lifetime and TLM samples for characterisation purposes. Uniform surfaces are seen at both the  $c$ -Si/ $a$ -Si:H( $i$ ) and the  $a$ -Si:H( $i$ )/polycrystalline Al interfaces. As opposed to the polycrystalline Al layer, an absence of diffraction contrast in the  $a$ -Si:H( $i$ ) layers suggests

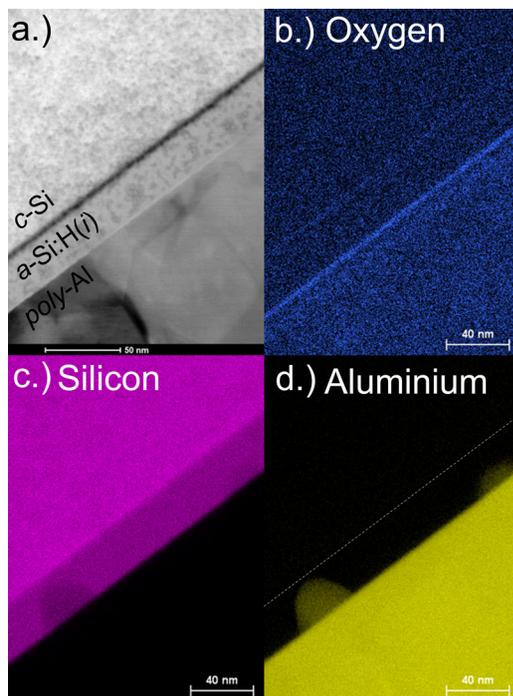


FIG. 4. (a) Bright field STEM image of the  $c$ -Si/ $a$ -Si:H( $i$ )/Al stack. EDX maps of the same region for (b) oxygen, (c) silicon, and (d) aluminium. The white dashed line in (d) represents the position of the  $c$ -Si/ $a$ -Si:H( $i$ ) interface.

that it remains in an amorphous state. The dark line at the  $c$ -Si/ $a$ -Si:H( $i$ ) interface is believed to be a measurement artifact rather than an interfacial species. Figures 4(b)–4(d) provide 2D EDX maps of the local O, Al and Si concentration through the entire depth of the sample ( $>100\ \text{nm}$ ), for the same region as shown in Figure 4(a). Figure 4(b) reveals that both interfaces host a thin unintentional oxide layer, the thicker of which is between Al and  $a$ -Si:H( $i$ ) films. The thin oxide at the  $c$ -Si/ $a$ -Si:H( $i$ ) interface may assist in maintaining amorphous growth during the high-temperature deposition, similar to the use of silicon-oxide deposition to prevent epitaxial film growth.<sup>25</sup> Local hemispherical protrusions can be seen originating from the aluminum layer in Figure 4(c) (which maps the Al concentration), suggesting partial spiking of the Al through the  $a$ -Si:H( $i$ ) film, which is supported by corresponding regions of lower silicon concentration in Figure 4(d). The higher temperature procedure ( $130^\circ\text{C}$ ) used for the STEM samples designate the obtained images as upper-limit representations of the aluminum spiking occurring in the TLM and lifetime samples.

### D. Conduction mechanisms

A lower limit protrusion depth of  $\sim 20\ \text{nm}$  can be estimated from the cross sectional images, implying that direct contact is most likely made to the  $c$ -Si surface for all thicknesses of  $a$ -Si:H( $i$ ) tested in the present study. These findings suggest that some conduction is achieved through a nano-scale partial contact structure. However, this conduction mechanism is unlikely to fully explain the thickness dependent  $\rho_c$  behavior observed for both the  $n^+$  and  $p^+$  surfaces. Instead, the results for  $\rho_c$  against  $a$ -Si:H( $i$ ) thickness suggest that the total conduction is the consequence of both direct contact through the aluminum protrusions, which has no strong dependence with interlayer thickness in the range of 0–15 nm, and a second parallel conduction mechanism with an exponential dependence on  $a$ -Si:H( $i$ ) thickness as illustrated in Figure 3. A candidate for the second mechanism, supported also in the literature,<sup>26</sup> is quantum-mechanical tunneling through the  $a$ -Si:H( $i$ ) layer; other conduction mechanisms, such as thermionic emission could not easily explain this trend. Starting from very thin  $a$ -Si:H( $i$ ) interlayers, a tunneling conduction mechanism could initially dominate the total conduction. The conductivity through this pathway would be expected to exponentially decrease (resistivity would exponentially increase) with increasing  $a$ -Si:H( $i$ ) interlayer thickness. At thicknesses of approximately 8 nm, the tunneling current becomes smaller than the direct conduction pathway through the aluminum protrusions, which dominates at thicknesses above this point, explaining the plateauing of  $\rho_c$ . It is expected that for  $a$ -Si:H( $i$ ) thicknesses greater than the protrusion depth (outside the measured range) the resistivity would be again higher.

In an effort to quantify the above suggestion of two parallel conduction pathways, the  $\rho_c$  trends in Figures 3(c) and 3(d) were each fitted with the inverse sum of two functions. One is a constant independent of thickness  $\rho_{c1}(t) = c$ , representative of spiking conduction; and the other function is

exponentially dependent on the thickness  $\rho_{c2}(t) = a \exp(bt)$ , representative of tunneling conduction. The second function  $\rho_{c2}(t)$ , can be compared to an approximate analytical expression for the inverse of the tunneling transmission coefficient  $T$  through a rectangular potential barrier given by<sup>27</sup>

$$\frac{1}{T(t)} = \exp\left(2t\sqrt{\frac{2m_{(e,h)}^*q\Phi_{eff(C,V)}}{\hbar^2}}\right) \propto \rho_c(t), \quad (1)$$

where  $\rho_c$  is inversely proportional to the tunneling transmission coefficient  $T$ .  $m_{(e,h)}^*$  is the tunneling effective electron or hole mass within the  $a$ -Si:H( $i$ ) layer,  $\hbar$  is the reduced Plank constant,  $q$  is the elementary charge, and  $\Phi_{eff(C,V)}$  is the effective barrier presented to conduction band electrons or valence band holes.

By equating the exponents of the modelled contact resistivity  $\rho_{c2}(t)$  and Eq. (1), it is possible to check if, as stated in Sec. III B, the differences in slope observed for the  $\rho_c(t)$  trends of the  $n^+$  and  $p^+$  contacts can be accounted for by differences in valence and conduction band offsets. The ratio of the fitted constants  $b$  of the  $p^+$  and  $n^+$  contact structures can be related to terms in Eq. (1) by

$$\left(\frac{b_{p^+}^2}{b_{n^+}^2} = 3.5\right) \approx \frac{m_h^*\Phi_{eff(V)}}{m_e^*\Phi_{eff(C)}}, \quad (2)$$

which is measured to be 3.5 in the present work. From trusted values in the literature presented in Figure 1, a  $\Phi_{eff(C)}$  value of  $\sim 0.34$  eV is calculated from the average height of the  $a$ -Si:H( $i$ ) conduction band above the  $c$ -Si conduction band. A similar analysis can be performed by comparison of the  $a$ -Si:H( $i$ ) and  $c$ -Si valence bands in Figure 1 to obtain a  $\Phi_{eff(V)}$  value of  $\sim 0.92$  eV. The values and validity of using electron and hole effective masses in  $a$ -Si:H( $i$ ) remain a contentious point;<sup>28</sup> however, if the assumption is made that the electron and hole effective masses are of a similar magnitude, then the calculated ratio in Eq. (2) is  $\sim 2.7$ , comparing reasonably well with the measured value of 3.5.

Although the measured exponential dependence of resistivity on thickness strongly suggest that tunneling through the  $a$ -Si:H( $i$ ) is a contributing mechanism to conduction, further studies are required to unequivocally confirm its role, given the complex nature of the contact and the aluminum— $a$ -Si:H( $i$ ) interaction and the uncertainties in the band offsets and effective masses.

## E. Consequences for solar cell performance

The above results demonstrate that whilst complete isolation of the aluminum and  $c$ -Si was not possible under these processing conditions, excellent contact characteristics were still achieved, particularly on the  $n^+$  surface. Included in Figures 3(c) and 3(d) as an approximate guide are lines (horizontal dashed lines) indicating appropriate  $\rho_c$  values for 5%, 10%, and 100% contact area, chosen in line with a total contact resistance  $R_c$  of  $0.05 \Omega \text{ cm}^2$ . For the phosphorus diffused contacts in Figure 3(c) it can be seen that the  $\rho_c$  limit for both the 5% and 10% contact fractions is exceeded in the

5–7 nm range where  $J_{oc}$  values still exhibit high recombination of  $\sim 500 \text{ fA/cm}^2$ . This situation can be improved by choosing full-area rear contacts, for which  $a$ -Si:H( $i$ ) thicknesses up to 15 nm are acceptable in terms of  $\rho_c$ . In this region  $J_{oc}$  values of  $\sim 40 \text{ fA/cm}^2$  are consistently attained for both 85 and 110  $\Omega/\square$   $n^+$  diffusions. Similarly, the boron diffused contacts in Figure 3(d) suggest that the optimum configuration is again a full area contact; however, in this instance,  $J_{oc}$  values in the 200–700  $\text{fA/cm}^2$  are to be expected—far higher than those on  $n^+$  surfaces.

For an estimation of the  $V_{oc}$  gain attained by applying the  $n^+$  contact to a solar cell, we introduce a comparison full-area deep phosphorus back surface region, which is known to have an optimum recombination parameter of  $\sim 300 \text{ fA/cm}^2$ . Using the optimum post-metallisation  $J_{oc}$  value of  $\sim 40 \text{ fA/cm}^2$  (with  $\sim 14$  nm of  $a$ -Si:H( $i$ )) found in this study, an upper-limit  $V_{oc}$  gain of  $\sim 50$  mV is calculated over an optimized full-area heavy phosphorus diffusion, using the method given in Ref 6. A similar analysis for the  $p^+$  surface provides less impressive results.

In summary, the results detailed in this paper present a simple modification to conventional homojunction solar cells which attains a high level of contact passivation. However, the sensitivity of the contact characteristics to temperature presents a technological challenge in ensuring low temperature back-end processing. Values in the literature suggest severe increases in recombination would result from temperatures in the vicinity of  $180^\circ\text{C}$ ,<sup>9</sup> and indeed, this study has shown that even temperatures as low as  $110^\circ\text{C}$  will affect device performance. The use of other metals with a higher  $a$ -Si:H( $i$ ) interaction temperature or an overlying conductive buffer layer may prove beneficial in improving contact stability.

## IV. CONCLUSION

As an alternative to an MIS contact,  $a$ -Si:H( $i$ ) was trialed as a passivating interlayer between heavily diffused phosphorus/boron surfaces and aluminum. The contact resistivity and contact recombination parameter were monitored as a function of  $a$ -Si:H( $i$ ) thickness in order to find the optimum. For both  $n^+$  and  $p^+$  diffusions a full area rear contact is found to be a suitable practical application of the passivated contact scheme developed in this paper. Superior majority carrier conductivity and surface passivation was found for the  $c$ -Si ( $n^+$ )/ $a$ -Si:H( $i$ )/Al contact with a  $\rho_c$  of  $< 0.05 \Omega \text{ cm}^2$  and a  $J_{oc}$  of  $\sim 40 \text{ fA/cm}^2$  for  $a$ -Si:H( $i$ ) thicknesses in the 12–15 nm range. These values translate to an upper-limit  $V_{oc}$  gain of  $\sim 50$  mV when compared to an optimised phosphorus back surface region. The  $c$ -Si ( $p^+$ )/ $a$ -Si:H( $i$ )/Al contact failed to achieve as low resistivity and recombination results, a larger valence band offset and larger minority carrier capture cross section area of interface defects are possible causes for this difference. STEM EDX analysis reveals that small aluminum protrusions through the  $a$ -Si:H( $i$ ) layer may contact the  $c$ -Si directly, thus contributing to conduction. The exponential trend of contact resistivity on interlayer thickness suggests that quantum-mechanical tunneling is a second conduction mechanism, which dominates at lower  $a$ -Si:H( $i$ ) thicknesses.

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