Intrinsic Silicon Buffer Layer Improves Hole-Collecting Poly-Si Passivating Contact

Jingxuan Kang,^{a)} Wenzhu Liu,^{a)} Thomas Allen, Michele De Bastiani, Xinbo Yang,
Stefaan De Wolf*

King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC),
Thuwal 23955-6900, Saudi Arabia

Abstract: Passivating contacts consisting of doped polycrystalline silicon (poly-Si) on a thin tunnel-oxide enable excellent operating voltages for crystalline silicon solar cells. However, hole-collecting contacts based on boron-doped poly-Si do not yet reach their full surface-passivation potential, likely due to boron diffusion during annealing. In this work, we show how the insertion of a thin intrinsic silicon buffer layer between the silicon oxide and poly-Si is effective in improving the contact passivation. By tailoring the microstructure of the buffer layer, the chemical passivation and contact resistivity are simultaneously significantly improved. On the device level, our buffer layer enables a ~30 mV open-circuit voltage enhancement and 1.4% absolute gain in power conversion efficiency.

a) These authors contributed equally to this work.

* stefaan.dewolf@kaust.edu.sa

Passivating contacts based on polycrystalline silicon (poly-Si) enable excellent open-circuit voltages (V_{oc}) and power conversion efficiencies (PCE) for crystalline silicon (c -Si) solar cells [1][2][3][4][5]. In 2018, a PCE of 26.1% was reported for a c -Si solar cell using such contacts in an interdigitated back contact (IBC) layout [6], approaching the world-record PCE of 26.7%, which utilises silicon heterojunction technology for its contact formation [7]. Poly-Si contacts usually feature a nanometer thin SiO_x layer in between the c -Si wafer and the (doped) poly-Si film to simultaneously enable excellent surface passivation and the collection of majority carriers. A major advantage of such contacts over their SHJ counterparts is their higher temperature resilience, offering processing-compatibility with current industrial solar cell manufacturing; devices that integrate hole-collecting poly-Si(p^+) contacts at the rear of conventional diffused-junction c -Si solar cells are anticipated to become the next mainstream industrial photovoltaic technology, replacing aluminum back surface field (BSF) and passivated emitter and rear emitter cell (PERC) technologies [1]. However, whereas electron-collecting poly-Si(n^+) contacts have already been demonstrated with excellent surface passivation [4][8][9], the case of their hole-collecting counterparts,

utilizing boron-doped poly-Si(p⁺), is hampered by relatively poor surface passivation [10][11]. Although additional hydrogenation treatments have been reported to further improve poly-Si(p⁺) contact passivation, with dark saturation current densities J_0 less than 5 fA/cm²[2][12], the relatively poor surface passivation afforded by poly-Si(p⁺) contacts compared to their n⁺ counterparts, remains a widely reported concern. Generally, Si dangling bonds present at the SiO_x/c-Si interface [13][14] and pinholes within the SiO_x formed during the annealing process [15][16][17] can limit the surface passivation of poly-Si contacts. Specifically, in the case of boron-doped poly-Si(p⁺) contacts, boron diffusion during high-temperature annealing, required to crystallize the deposited amorphous silicon films into poly-Si, may additionally create a high density of hole-trapping, boron-induced oxygen-vacancy states in the SiO_x layer, as well as strain in the contact structure leading to pinhole formation, all of which strongly limit the surface passivation [15][18][19][20][21][22][23][24].

To improve the surface passivation in a similar contact structure, Nogay *et al.* inserted a thin intrinsic amorphous silicon (a-Si) buffer layer between a SiC(p⁺) and SiO_x layer [2][25]. They reported that the buffer layer boosts the SiC(p)/SiO_x/c-Si contact passivation by mitigating the chemical reaction of SiO_x with carbon from the SiC_x(p) layer as well as limiting the dopant (B⁺) accumulation around the SiO_x layer. In this work, to address the details of passivation degeneration by boron-diffusion, we insert a thin intrinsic hydrogenated amorphous silicon [*a*-Si:H(i)] buffer layer with a tailored microstructure between the *a*-Si:H(p⁺) and SiO_x layers. Subsequently, the high-temperature annealing process transforms the *a*-Si:H stack to the poly-Si phase, forming hole-collecting poly-Si passivating contacts. We find that *a*-Si:H(i) with a moderate mass density is the most suitable buffer layer for achieving high-quality poly-Si(p⁺) contacts, evidenced by a lower surface recombination velocity and contact resistance. Moreover, this work also investigates the effects of B⁺ on the SiO_x structure and residual silicon surface defects on the contact passivation. On the device level, insertion of this buffer leads to gains in of 1.4% in absolute PCE compared to our reference solar cell.

Figure 1. (a) Si-H stretching-mode absorptions of as-deposited *a*-Si:H(i) buffers, labeled as porous, medium and dense, characterized by Fourier-transform infrared (FTIR) spectroscopy. (b) Raman-spectroscopy peak full width at half maximum (FWHM) of the porous, medium, and dense *a*-Si:H(i) buffer layers at wavenumber 518cm⁻¹ and 500cm⁻¹ respectively after high-temperature annealing.

For the experiments, double-side polished *c*-Si floatzone (FZ) *n*-type (100) *c*-Si wafers (280±20μm, 1-5 Ω·cm) were dipped into a 5% HF solution for 1 minute to remove the surface native oxide, followed by rinsing in de-ionized water. Next, the wafers were immersed in a boiling nitric acid solution (concentration >69%) for 15mins for tunneling oxide growth (~1.5 nm). Subsequently, stacks of 12 nm *a*-Si:H(i) and 30 nm *a*-Si:H(p⁺) films were successively deposited by plasma-enhanced chemical vapor deposition (PECVD) at 200°C (Oxford Plasma System100; Octopus PECVD, Indeotec). For tailoring the *a*-Si:H(i) microstructure, the Ar/SiH₄ or H₂/SiH₄ gas flow ratios were gradually increased. Depending on these ratios, we found the density of the resulting *a*-Si:H(i) films, inferred from the microstructure factor *R* (discussed below), to be “porous” (pure SiH₄, 200 sccm); “medium” (SiH₄/Ar 20/475sccm); and “dense” (SiH₄/H₂: 25/800 sccm). For comparison, a similar structure without an *a*-Si:H(i) buffer layer was also fabricated. All samples were then transferred into a tube furnace at room temperature, which was then increased to 850°C with a heating rate of 10°C/min. The samples were then held at a plateau of 850°C for 30 min, followed by passive cooling to room temperature. The full annealing process was performed in a pure N₂ atmosphere without subsequent hydrogenation of the films. The minority carrier lifetime of the annealed samples was measured by a Sinton WCT-120 instrument, and the boron profiles were probed by secondary ion mass spectrometry (SIMS) with an O⁻ ion source. Contact resistivities were extracted by the Cox and Strack method [26]. 300nm full area aluminum is deposited at the backside of Poly-Si(p⁺)/SiOx/*c*-Si(p) stacks, and aluminum circles (300nm) that featured with 0.8mm, 0.6mm, 0.4mm, 0.3mm, 0.25mm, 0.2mm and 0.15mm diameters are deposited at the surface of poly-Si(p⁺). To characterize the microstructure of the *a*-Si:H(i) buffer layer before annealing, Fourier-transform infrared (FTIR) spectra of the porous,

medium, and dense films were measured in transmission mode. The annealed intrinsic buffer films were characterized by Raman spectroscopy (NTEGRA Spectra, NT-MDT Spectrum Instruments) and conductive atomic force microscopy was performed to measure the current signal flows through the poly-Si(p⁺) contact with the medium buffer layer under 500mV bias voltage. Finally, we tested our buffer layers on device level by fabricating two-sided poly-Si passivating-contact solar cells. For this, as before, thin SiO_x films (~1.5nm) were wet-chemically grown. Then a 30 nm *a*-Si:H(n⁺) film and either a 30 nm *a*-Si:H(p⁺) or an *a*-Si:H(i)/*a*-Si:H(p⁺) stack were deposited onto these SiO_x films by PECVD on the respective wafer sides. After film deposition, the samples were annealed in a tube furnace. Next, 80nm and 120nm of indium tin oxide (ITO) was sputtered on the front and rear side, respectively. Finally, a full area silver contact was sputtered on to the rear side of the solar cells, and silver paste was screen printed to realize the front grid followed by 15 minutes of curing at 200°C.

As stated, the microstructure of *a*-Si:H films can be inferred from the microstructure factor R , which is the ratio of integrated absorption intensity mode around 2080 cm⁻¹ to the sum of integrated absorption intensities of modes around 2080 cm⁻¹ and 2010 cm⁻¹.

$$R = \frac{[2080]}{[2010] + [2080]}$$

Fig. 1(a) show Si-H FTIR spectra of the porous, medium and dense *a*-Si:H(i) films. The porous and dense films show pronounced stretching modes at ~2080 cm⁻¹ and ~2010 cm⁻¹ respectively. With $R = 0.11$ and 0.64, their microstructures are found to be porous and dense, respectively. The moderate R value of 0.48 for our ‘medium’ *a*-Si:H(i) film indicates it effectively has a medium mass density, *i.e.*, between porous and dense [27][28]. Fig. 2(a) shows the B⁺ depth profile, acquired by SIMS, of the annealed poly-Si(p⁺)/c-Si interface with and without *a*-Si:H(i) buffer layers. Although the control sample without a buffer layer has a thinner poly-Si(p⁺) layer (20nm) than those with the buffer layer (40nm), the control sample has the highest interfacial B⁺ density. It is seen that a high density of boron atoms aggregates at the SiO_x tunneling layer, which likely ‘poisons’ the interface, impairing effective passivation. Fig. 2(a) shows that the porous 12 nm *a*-Si:H(i) buffer effectively hinders the diffusion of boron atoms. As a consequence, the B⁺ density becomes lower at the SiO_x/c-Si interface, compared to the control sample. Similarly, the dense *a*-Si:H(i) buffer layer also impedes the diffusion of boron atoms, improving the interface passivation as well. Interestingly, the medium *a*-Si:H(i) acts as the best buffer layer, displaying the lowest interfacial boron density.

Figure 2. (a) Boron density profile measured by SIMS for the poly-Si(p⁺)/SiO_x/c-Si contact interfaces with and without 12 nm buffer layers. (b) The minority carrier lifetime of control, Porous, Medium and Dense symmetric contacts at $1 \times 10^{15} \text{ cm}^{-3}$ injection level respectively. (c) Schematic of poly-Si(p⁺)/SiO_x/c-Si contact structure with pinhole. (d) c-AFM image of poly-Si(p⁺) contact without buffer layer under 500mV applied voltage.

In *a*-Si:H(p⁺) films, the boron-doped sites experience a high strain due to bond-length fluctuations [29]. During high-temperature annealing B–Si bonds are susceptible to rupture, upon which the small boron atoms can thermally diffuse in the amorphous network, which can explain the accumulation of boron atoms in the SiO_x layer [30]. For the porous *a*-Si:H(i), high-temperature annealing leads to drastic internal-void collapse and hydrogen effusion from the *a*-Si:H matrix [31][32]. Simultaneously to the hydrogen effusion, large amounts of boron atoms find vacancies to diffuse to the buffer layer, and finally a portion of them may reach the *c*-Si surface. Refs. [12] and [13] described similar phenomena, where violent hydrogen effusion and slow crystallization facilitate the diffusion of boron atoms, and the creation of a high density of Si dangling bonds. These vacant states assist boron migration in *a*-Si:H [30]. Boron atoms show a lower accumulation in our buffer layers of medium density due to its more ordered structure and lower hydrogen content [30], in agreement with the fewer detected boron atoms at the SiO_x/c-Si interface, as shown in Fig.

2(a). We propose that the higher ordered microstructure of the dense α -Si:H buffer results in the formation of a high density of small poly-Si grains during annealing [11][15][16]. Such small poly-Si grains lead to high defect and grain-boundary densities, providing effective diffusion paths for boron atoms, as their diffusion coefficient is higher along the grain boundaries than inside poly-Si grains [33][34][35][36]. Figure 1(b) illustrates the Raman spectroscopy peak full width at half maximum (FWHM) around 518 cm^{-1} and 500 cm^{-1} of our porous, medium and dense buffers after annealing. These Raman peaks corresponds to c-Si and the outer shell of grain cores, which consists of near-surface fine size crystalline phases with irregular shapes. An increase in FWHM indicates a reduction in average poly-Si grain size [37][38][39][40]. Compared with the dense buffer layer, the medium buffer layer results in slightly larger poly-Si grains with a relatively lower grain-boundary density, and hence fewer channels for boron diffusion. In figure 2(a), similar interfacial boron densities are found in the porous and dense buffer layers. This suggests that the diffusion of boron atoms can be represented by a competition between vacancy-assisted and grain boundary migration, and the porous and dense buffer layers have a similar boron diffusion rate during the annealing process.

Fig. 2(b) displays the minority carrier lifetime of symmetric poly-Si(p^+) contacts with and without buffer layers. All the poly-Si(p^+) contacts with buffer layers exhibit higher minority carrier lifetimes than that of the control sample, demonstrating that impeding boron migration via buffer layers indeed improves the poly-Si(p^+) contact passivation. Clearly, the best passivation, with minority carrier lifetime ~ 1.6 ms and $J_0 \sim 21 \text{ fA.cm}^{-2}$, is obtained using the medium buffers, likely due to the reduction in boron accumulation in the SiO_x tunneling layer, which in turn leads to a lower c-Si surface defect density and reduced pinhole area, as we discuss below. In terms of porous and dense buffers, a very similar boron density around SiO_x is measured, which is consistent with their similar minority carrier lifetimes in fig. 2(d). The main reason for this B^+ density difference around the SiO_x layer is the diffusion-coefficient variation in different structures of buffer layers. As discussed in the last paragraph, the porous buffer suffers from violent hydrogen effusion and slow crystallization processes that create a high density of sites for boron atom migration during the annealing process. Thanks to a more optimal hydrogen content and poly-silicon grain size, the medium buffer obtains the minimum boron diffusion coefficient and, consequently, the lowest interfacial B^+ density. In addition to boron-induced defects in the SiO_x , silicon dangling bonds in the pinhole area also need to be considered as a contribution for the poly-Si(p^+) contact-passivation degeneration. Figure 2(d) shows the areal density of pinholes formed after annealing, determined by c-AFM, and the schematic of figure 2(c) depicts the interfacial structure with a pinhole. Strained and dangling bonds are generated during the annealing process due to boron incorporation in SiO_x , which contributes to pinhole formation. The conclusion from reference [41] that the pinhole density increases with B^+ doping concentration in the SiC(p^+) as well as increased annealing temperature are consistent with this conclusion.

An increasing pinhole area degrades the contact passivation because the associated silicon dangling bonds are located between the poly-Si(p⁺)/c-Si contacts. We, therefore, hypothesize that the pinhole density and interfacial boron density are the main contributions limiting the poly-Si(p⁺) contact minority carrier lifetime.

Notably, the addition of intrinsic buffers is also beneficial from the majority-carrier perspective: when the medium buffer layer is used to fabricate poly-Si(p⁺) contacts, an ohmic contact with $\sim 3 \text{ m}\Omega/\text{cm}^2$ contact resistivity is obtained, which is an order of magnitude lower than for the reference structure [see Fig. 3(a) and (b)]. We propose that a lower interfacial defect density, likely resulting in a reduced pinning of the Fermi-level, is the major reason for this improvement. Indeed, for the poly-Si(p⁺)/SiO_x/c-Si contact without a buffer layer, as Fig 2(a) demonstrates, a higher density of boron atoms has accumulated around the SiO_x layer; part of the boron atoms have penetrated and accumulated into SiO_x layer during high-temperature annealing [20][22][42]. Strained and dangling bonds are generated during the annealing process due to boron incorporation in SiO_x. Here, arguably the most probable defect which plays a role in the poly-Si(p⁺)/SiO_x/c-Si(p) contact-resistivity variation is the boron-decorated oxygen vacancy within the amorphous SiO_x films [18][19] [43][44]. The O-deficient point defects are energetically positioned at about $E-E_i=0.05 \text{ eV}$ within the SiO_x layer [18][19][23][24][43][45]. In amorphous SiO_x films that coat *c*-Si surfaces, these defects act as donor-like surface states within the *c*-Si band gap, resulting in Fermi-level pinning and thereby inducing a transport barrier for holes with a certain energy [23][45][46][47]. To further confirm this defect-induced phenomenon, we simulated the band alignment of poly-Si(p⁺)/SiO_x/c-Si(p) contacts with a range of different interfacial O-deficient point-defect densities. Fig 3(c) shows the band alignments with different interfacial defects densities, D_{it} . Obviously, a high D_{it} induces a high transport barrier for holes, positioned at the valence band maximum. Therefore, we conclude that the buffer layer effectively reduces the contact resistance for hole transport by suppressing the boron-induced defect density.

Figure 3. I-V curves of different contact areas on poly-Si(p⁺)/SiO_x/c-Si(p) contact without (a) and with (b) buffer layer. (c) AFORS-HET v2.5 simulated band bending at poly-Si(P⁺)/SiO_x/c-Si(P) interface with variable D_{it} from 1.5×10^{10} cm⁻² to 1.5×10^{13} cm⁻².

Next, we test the poly-Si(p⁺) with buffer-layer contact by fabricating 4 cm² c-Si(n) solar cells, as sketched in Fig. 4(a). The device features planar surfaces with a front junction. Based on this structure, first, we did device simulations for which different O-deficient defect densities at the SiO_x/c-Si(n) interface. Fig 4(b) shows the simulated J-V characteristics, from which it can be seen that, expectedly, a higher interfacial D_{it} hinders a high V_{oc} and fill factor, FF . Indeed, an increase in D_{it} results in interface recombination, obviously detrimentally affecting the V_{oc} and voltage at the maximum power point, and so decreasing the FF . Moreover, $D_{it} > 1.5 \times 10^{12}$ cm⁻² results in Fermi-level pinning, inducing a (thermionic) energy barrier for hole transport, further affecting the FF . We note that in addition to donor-like O-deficient point defects, acceptor-like defects have also been reported in the SiO_x/c-Si system [15][18][48], in which case our simulations find similar trends as given in Fig.4 (b), again due to Fermi-level pinning (data not shown). Figure 4(c) shows the illuminated J-V curves of experimental solar cells with and without a buffer layer. In agreement with the simulated results, via buffer layer insertion, the device PCE significantly improves from 16.8% to 18.2%, thanks to increases in V_{oc} and FF . This is typical behavior expected from improved

chemical interface-passivation and is consistent with the lifetime results of Fig. 2 (b) [49][50][51]. Our solar cells were mainly fabricated as a proof-of-concept test platform for our poly-Si contacts; a PCE of >22% can be expected if the wafer is textured as in state-of-the-art devices.

Figure 4. (a) Device sketch of poly-Si passivating contact solar cell with buffer layer. (b) Simulated J-V curves against D_{it} in AFORS-HET v2.5. (c) J-V curves of devices on planar c-Si wafers employing p-type poly-Si contacts with and without buffer layer

To conclude, we propose inserting a thin intrinsic silicon buffer layer between the tunnel oxide and poly-Si(p⁺) for efficient hole-collecting passivating contacts to simultaneously improve the interface passivation and contact resistivity of silicon solar cells. During high temperature annealing, the *a*-Si:H(i) buffer layer prevents boron migration from the poly-Si(p⁺) film to the SiO_x/c-Si interface, thereby improving the poly-Si(p⁺)/SiO_x/c-Si interface passivation. FTIR, SIMS, and minority lifetime investigations demonstrate that medium density intrinsic *a*-Si:H films are the most suitable candidates for the boron diffusion buffer layer. Finally, the passivating-contact solar cell performance confirms that employment of a medium-density intrinsic *a*-Si:H buffer results in >1% gains in absolute PCE improvement.

Acknowledgments

This work was supported by funding from King Abdullah University of Science and Technology (KAUST) Office of Sponsored Research (OSR) under award no. OSR-CRG URF/1/3383.

Reference

- [1] T. G. Allen, J. Bullock, X. Yang, A. Javey, and S. De Wolf, "Passivating contacts for crystalline silicon solar cells," *Nat. Energy*, pp. 1–15, 2019.
- [2] A. Ingenito *et al.*, "A passivating contact for silicon solar cells formed during a single firing thermal annealing," *Nat. Energy*, vol. 3, no. 9, p. 800, 2018.
- [3] G. Nogay *et al.*, "Interplay of annealing temperature and doping in hole selective rear contacts based on silicon-rich silicon-carbide thin films," *Sol. Energy Mater. Sol. Cells*, vol. 173, pp. 18–24, 2017.
- [4] F. Feldmann, M. Bivour, C. Reichel, M. Hermle, and S. W. Glunz, "Passivated rear contacts for high-efficiency n-type Si solar cells providing high interface passivation quality and excellent transport characteristics," *Sol. Energy Mater. Sol. Cells*, vol. 120, pp. 270–274, 2014.
- [5] U. Römer *et al.*, "Recombination behavior and contact resistance of n+ and p+ poly-crystalline Si/mono-crystalline Si junctions," *Sol. Energy Mater. Sol. Cells*, vol. 131, pp. 85–91, 2014.
- [6] F. Haase *et al.*, "Laser contact openings for local poly-Si-metal contacts enabling 26.1%-efficient POLO-IBC solar cells," *Sol. Energy Mater. Sol. Cells*, vol. 186, pp. 184–193, 2018.
- [7] K. Yoshikawa *et al.*, "Exceeding conversion efficiency of 26% by heterojunction interdigitated back contact solar cell with thin film Si technology," *Sol. Energy Mater. Sol. Cells*, vol. 173, pp. 37–42, 2017.
- [8] A. Moldovan, F. Feldmann, M. Zimmer, J. Rentsch, J. Benick, and M. Hermle, "Tunnel oxide passivated carrier-selective contacts based on ultra-thin SiO₂ layers," *Sol. Energy Mater. Sol. Cells*, vol. 142, pp. 123–127, 2015.
- [9] D. Yan, A. Cuevas, J. Bullock, Y. Wan, and C. Samundsett, "Phosphorus-diffused polysilicon contacts for solar cells," *Sol. Energy Mater. Sol. Cells*, vol. 142, pp. 75–82, 2015.
- [10] F. Feldmann, J. Schön, J. Niess, W. Lerch, and M. Hermle, "Studying dopant diffusion from Poly-Si passivating contacts," *Sol. Energy Mater. Sol. Cells*, vol. 200, p. 109978, 2019.
- [11] U. Römer *et al.*, "Ion implantation for poly-Si passivated back-junction back-contacted solar cells," *IEEE J. Photovoltaics*, vol. 5, no. 2, pp. 507–514, 2015.
- [12] S. Mack, J. Schube, T. Fellmeth, F. Feldmann, M. Lenes, and J. Luchies, "Metallisation of boron-doped polysilicon layers by screen printed silver pastes," *Phys. status solidi (RRL)—Rapid Res. Lett.*, vol. 11, no. 12, p. 1700334, 2017.
- [13] J. H. Stathis and E. Cartier, "Atomic hydrogen reactions with P b centers at the (100) Si/SiO₂ interface," *Phys. Rev. Lett.*, vol. 72, no. 17, p. 2745, 1994.

- [14] A. Stirling, A. Pasquarello, J.-C. Charlier, and R. Car, "Dangling Bond Defects at Si– SiO₂ Interfaces: Atomic Structure of the P b 1 Center," *Phys. Rev. Lett.*, vol. 85, no. 13, p. 2773, 2000.
- [15] W. Liu *et al.*, "Poly-Silicon Passivating Contacts for Silicon Solar Cells: Interface Passivation and Carrier Transport Mechanism," *ACS Appl. Energy Mater.*, 2019.
- [16] I. R. C. Post, P. Ashburn, and G. R. Wolstenholme, "Polysilicon emitters for bipolar transistors: a review and re-evaluation of theory and experiment," *IEEE Trans. Electron Devices*, vol. 39, no. 7, pp. 1717–1731, 1992.
- [17] G. R. Wolstenholme, N. Jorgensen, P. Ashburn, and G. R. Booker, "An investigation of the thermal stability of the interfacial oxide in polycrystalline silicon emitter bipolar transistors by comparing device results with high-resolution electron microscopy observations," *J. Appl. Phys.*, vol. 61, no. 1, pp. 225–233, 1987.
- [18] R. A. B. Devine, *The physics and technology of amorphous SiO₂*. Springer Science & Business Media, 2012.
- [19] M. Offenberger, M. Maier, R. Meyer, and P. Balk, "Nature of defects in P-and B-doped SiO₂," *J. Vac. Sci. Technol. A Vacuum, Surfaces, Film.*, vol. 4, no. 3, pp. 1009–1012, 1986.
- [20] K. Uwasawa, T. Mogami, T. Kunio, and M. Fukuma, "Scaling limitations of gate oxide in p/sup+/polysilicon gate MOS structures for sub-quarter micron CMOS devices," in *Proceedings of IEEE International Electron Devices Meeting*, 1993, pp. 895–898.
- [21] T. Yamamoto, K. Uwasawa, and T. Mogami, "Bias temperature instability in scaled p/sup+/polysilicon gate p-MOSFET's," *IEEE Trans. Electron Devices*, vol. 46, no. 5, pp. 921–926, 1999.
- [22] D. A. Buchanan, "Scaling the gate dielectric: materials, integration, and reliability," *IBM J. Res. Dev.*, vol. 43, no. 3, pp. 245–264, 1999.
- [23] A. Yokozawa, A. Oshiyama, Y. Miyamoto, and S. Kumashiro, "Oxygen vacancy with large lattice distortion as an origin of leakage currents in SiO₂," in *International Electron Devices Meeting. IEDM Technical Digest*, 1997, pp. 703–706.
- [24] P. E. Blöchl, "First-principles calculations of defects in oxygen-deficient silica exposed to hydrogen," *Phys. Rev. B*, vol. 62, no. 10, p. 6158, 2000.
- [25] G. Nogay *et al.*, "Silicon-rich silicon carbide hole-selective rear contacts for crystalline-silicon-based solar cells," *ACS Appl. Mater. Interfaces*, vol. 8, no. 51, pp. 35660–35667, 2016.
- [26] R. H. Cox and H. Strack, "Ohmic contacts for GaAs devices," *Solid. State. Electron.*, vol. 10, no. 12, pp. 1213–1218, 1967.

- [27] E. Bhattacharya and A. H. Mahan, "Microstructure and the light-induced metastability in hydrogenated amorphous silicon," *Appl. Phys. Lett.*, vol. 52, no. 19, pp. 1587–1589, 1988.
- [28] K. Sharma, A. Branca, A. Illiberi, F. D. Tichelaar, M. Creatore, and M. C. M. van de Sanden, "On the effect of the amorphous silicon microstructure on the grain size of solid phase crystallized polycrystalline silicon," *Adv. Energy Mater.*, vol. 1, no. 3, pp. 401–406, 2011.
- [29] I. Santos, P. Castrillo, W. Windl, D. A. Drabold, L. Pelaz, and L. A. Marqués, "Self-trapping in B-doped amorphous Si: Intrinsic origin of low acceptor efficiency," *Phys. Rev. B*, vol. 81, no. 3, p. 33203, 2010.
- [30] S. Mirabella *et al.*, "Mechanism of boron diffusion in amorphous silicon," *Phys. Rev. Lett.*, vol. 100, no. 15, p. 155901, 2008.
- [31] W. Liu *et al.*, "Characterization of microvoids in thin hydrogenated amorphous silicon layers by spectroscopic ellipsometry and Fourier transform infrared spectroscopy," *Scr. Mater.*, vol. 107, pp. 50–53, 2015.
- [32] B. Macco *et al.*, "Correlating the silicon surface passivation to the nanostructure of low-temperature a-Si: H after rapid thermal annealing," *J. Appl. Phys.*, vol. 122, no. 3, p. 35302, 2017.
- [33] A. D. Buonaquisti, W. Carter, and P. H. Holloway, "Diffusion characteristics of boron and phosphorus in polycrystalline silicon," *Thin Solid Films*, vol. 100, no. 3, pp. 235–248, 1983.
- [34] B. Han *et al.*, "Phosphorus and boron diffusion paths in polycrystalline silicon gate of a trench-type three-dimensional metal-oxide-semiconductor field effect transistor investigated by atom probe tomography," *Appl. Phys. Lett.*, vol. 107, no. 2, p. 23506, 2015.
- [35] S. Jin, K. S. Jones, M. E. Law, and R. Camillo-Castillo, "B segregation to grain boundaries and diffusion in polycrystalline Si with flash annealing," *J. Appl. Phys.*, vol. 111, no. 4, p. 44508, 2012.
- [36] W. A. Rausch, R. F. Lever, and R. H. Kastl, "Diffusion of boron into polycrystalline silicon from a single crystal source," *J. Appl. Phys.*, vol. 54, no. 8, pp. 4405–4407, 1983.
- [37] X. Jia *et al.*, "Accurate analysis of the size distribution and crystallinity of boron doped Si nanocrystals via Raman and PL spectra," *RSC Adv.*, vol. 7, no. 54, pp. 34244–34250, 2017.
- [38] L. Houben, M. Luysberg, P. Hapke, R. Carius, F. Finger, and H. Wagner, "Structural properties of microcrystalline silicon in the transition from highly crystalline to amorphous growth," *Philos. Mag. A*, vol. 77, no. 6, pp. 1447–1460, 1998.
- [39] A. Achiq *et al.*, "Effects of prior hydrogenation on the structure and properties of thermally nanocrystallized silicon layers," *J. Appl. Phys.*, vol. 83, no. 11, pp. 5797–5803, 1998.
- [40] T. Jawhari, "Micro-Raman spectroscopy of the solid state: applications to semiconductors and

- thin films,” *Analysis*, vol. 28, no. 1, pp. 15–21, 2000.
- [41] G. Nogay, “Full-Area Passivating Contacts with High and Low Thermal Budgets: Solutions for High Efficiency c-Si Solar Cells,” EPFL, 2018.
 - [42] B. Y. Kim, I. M. Liu, H. F. Luan, M. Gardner, J. Fulford, and D. L. Kwong, “Impact of boron penetration on gate oxide reliability and device lifetime in p/sup+/-poly PMOSFETs,” in *1997 IEEE International Reliability Physics Symposium Proceedings. 35th Annual*, 1997, pp. 287–291.
 - [43] R. B. Fair, “Physical models of boron diffusion in ultrathin gate oxides,” *J. Electrochem. Soc.*, vol. 144, no. 2, p. 708, 1997.
 - [44] M. Offenbergh, T. Johansson, M. Aslam, and P. Balk, “Electron traps in B⁺-implanted SiO₂,” *Phys. B+ C*, vol. 129, no. 1–3, pp. 240–244, 1985.
 - [45] E. H. Poindexter and W. L. Warren, “Paramagnetic Point Defects in Amorphous Thin Films of SiO₂ and Si₃N₄: Updates and Additions,” *J. Electrochem. Soc.*, vol. 142, no. 7, pp. 2508–2516, 1995.
 - [46] P. M. Lenahan and P. V Dressendorfer, “Hole traps and trivalent silicon centers in metal/oxide/silicon devices,” *J. Appl. Phys.*, vol. 55, no. 10, pp. 3495–3499, 1984.
 - [47] S. Lombardo, J. H. Stathis, B. P. Linder, K. L. Pey, F. Palumbo, and C. H. Tung, “Dielectric breakdown mechanisms in gate oxides,” *J. Appl. Phys.*, vol. 98, no. 12, p. 12, 2005.
 - [48] B. Stegemann *et al.*, “Ultra-thin silicon oxide layers on crystalline silicon wafers: Comparison of advanced oxidation techniques with respect to chemically abrupt SiO₂/Si interfaces with low defect densities,” *Appl. Surf. Sci.*, vol. 395, pp. 78–85, 2017.
 - [49] M. Reusch, M. Bivour, M. Hermle, and S. W. Glunz, “Fill factor limitation of silicon heterojunction solar cells by junction recombination,” *Energy Procedia*, vol. 38, pp. 297–304, 2013.
 - [50] D. Adachi, J. L. Hernández, and K. Yamamoto, “Impact of carrier recombination on fill factor for large area heterojunction crystalline silicon solar cell with 25.1% efficiency,” *Appl. Phys. Lett.*, vol. 107, no. 23, p. 233506, 2015.
 - [51] L. Shen, F. Meng, and Z. Liu, “Roles of the Fermi level of doped a-Si: H and band offsets at a-Si: H/c-Si interfaces in n-type HIT solar cells,” *Sol. Energy*, vol. 97, pp. 168–175, 2013.