Band-gap profiling in amorphous silicon–germanium solar cells

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Profiled buffer layers at the interfaces of amorphous silicon–germanium (*a*-SiGe:H) solar cells are routinely used to avoid band-gap discontinuities and high-defect densities at the p/i and i/n interfaces. It is shown that such profiled *a*-SiGe:H buffer layers can be replaced by a constant band-gap *a*-Si:H buffer, an inverse profiled *a*-SiGe:H buffer, or even a 3-nm-thin (δ) buffer at some distance away from the interface without losses in the open-circuit voltage V_{OC} and fill factor while maintaining the same short current density j_{SC}. In view of these results, common model assumptions for *a*-SiGe:H solar cells have to be revised. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1456548]

For amorphous silicon (*a*-Si:H) based stacked solar cells, the classical red absorber is amorphous silicon–germanium (*a*-SiGe:H), which has a lower optical band gap (depending on the Ge concentration) than compared to *a*-Si:H. These solar cells in $p-i-n$ (or $n-i-p$) configuration usually contain *a*-Si:H p and n layers. Consequently, there is a band-gap discontinuity at the p/i and i/n interfaces. Since the defect density of *a*-SiGe:H increases with decreasing optical band gap (i.e., increasing Ge content), one expects a high-defect density at the p/i and i/n interfaces, which will adversely affect the internal electric field and the carrier collection, resulting in poor open-circuit (OC) voltages V_{OC} and fill factors (FFs). Additionally, in the picture of the so-called defect pool model, the defect density near the interfaces is strongly enhanced due to the position of the Fermi level.[1] Therefore, considerable effort has been made to counteract these effects by smooth band-gap grading at the interfaces and, in fact, even throughout the entire *a*-SiGe:H absorber layer.[2–6]

In contrast to these concepts, we present an alternative approach where only the band-gap design in the interface region within a distance of 15 nm to the p/i and i/n interfaces is modified while the intrinsic *a*-SiGe:H absorber layer is kept at a constant band gap (1.5 eV). It will be shown that the profiled *a*-SiGe:H buffer layers at the p/i and i/n interfaces can be replaced by *a*-Si:H buffer layers, or even by an inversely profiled *a*-SiGe:H buffer layer without any loss in FF and V_{OC}. Furthermore, the influence of the position of a 3-nm-thin buffer layer (with various band gaps) on the solar cell performance is investigated. This leads to surprising insights into the role of interface layers.

All cells were deposited in a multichamber UHV glow discharge system with diode-type electrode configuration and the substrate located at the unpowered electrode (substrate size 100 cm^2; 2 cm electrode spacing). Si_2H_6, GeH_4, and H_2 are used as process gases. The deposition conditions were: pressure 93 Pa, power density 35 mW/cm^2, substrate temperature 200 °C. All cells were deposited on textured SnO_2 (ASAHI, type "U") and had Ag backreflectors. The cell area was 1 cm^2. The *a*-SiGe:H *i* layer in this test cell structure had a constant band gap of $E_G = 1.5$ eV. This layer was 54–66 nm thick and was not optimized to deliver high-current densities. This is not necessary for the present study because the main effects are expected for the V_{OC} and the FF, and thus a high level of V_{OC} and FF as a starting point is required to show the general trends. A-Si:H and profiled *a*-SiGe:H buffer layers with different thicknesses were applied. The band-gap steps were realized by changing the respective gas flows without plasmastop. The gas exchange times are in the order of a few seconds and the resulting nonintentional profilings are in the range of only a few Å and can be neglected. The details of the interface designs are shown in the following schematic diagrams together with the results. The current density–voltage ($J-V$) parameters of the cells were measured under red light using a 590 nm cut-on filter to simulate the light exposure of the bottom cell in a tandem stack.

In a first experiment, we compared cell structures with (a) normally profiled *a*-SiGe:H buffers, (b) *a*-Si:H buffers using various thicknesses for the buffer layers, and (c) inversely profiled *a*-SiGe:H buffers (Fig. 1). In cases (a) and (b), the thickness of the two buffer layers was simultaneously increased from 0 to 12 nm. To achieve similar current densities [short current density (SC)] j_{SC} for cases (a) and (b),

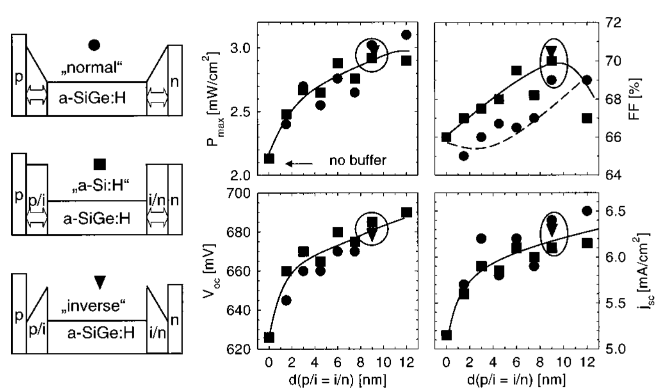

FIG. 1. Comparison between *a*-SiGe:H solar cells with *a*-Si:H buffer layers and the profiled *a*-SiGe:H buffer at the p/i and i/n interfaces. The values for the FF and V_{OC} are measured as a function of the thickness of the interface layer. $d(p/i) = d(i/n)$. Shown are cells with the *a*-Si:H buffer (■), cells with the normally profiled *a*-SiGe:H buffer (●) and a cell with the inversely profiled *a*-SiGe:H buffer (▼).

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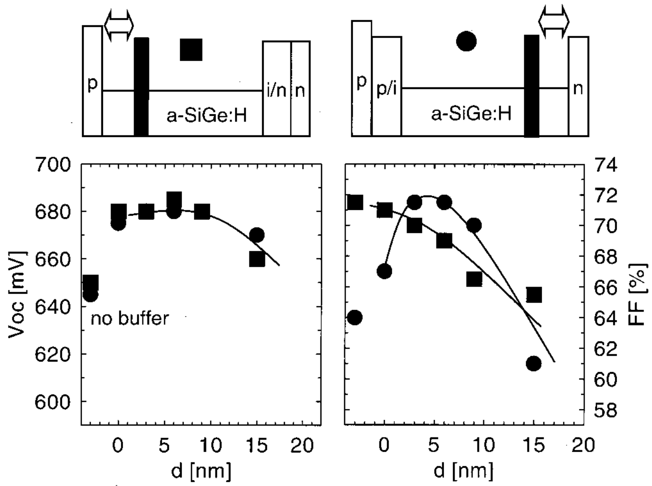

FIG. 2. Influence of a 3-nm-thick *a*-Si:H buffer layer at the p/i (■) and i/n interfaces (●). The values for the FF and V_{OC} are measured as a function of position d of the buffer layer with respect to the next doped layer. The optical band gap of the *a*-SiGe:H absorber layer is constant at 1.5 eV. Negative values for d indicate no buffer layer.

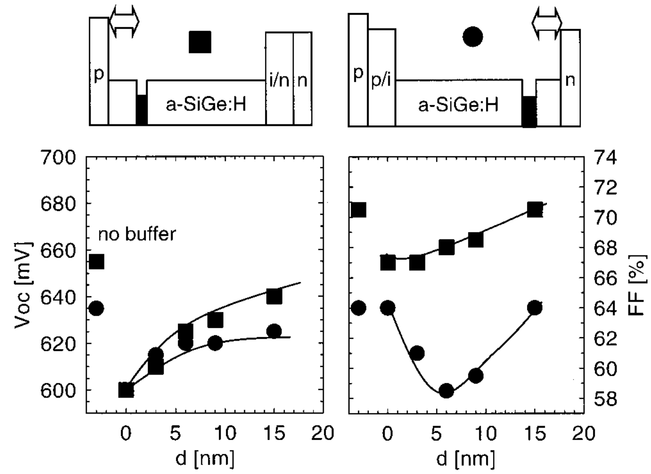

FIG. 3. Influence of a 3-nm-thick *a*-SiGe:H buffer layer (1.4 eV) at the p/i (■) and i/n interfaces (●). The values for the FF and V_{OC} are measured as a function of position d of the buffer layer with respect to the next doped layer. The optical band gap of the *a*-SiGe:H absorber layer is constant at 1.5 eV. Negative values for d indicate no buffer layer.

the *i*-layer thickness had to be adjusted to take care of the increased absorption in the profiled buffer which contains *a*-SiGe:H.

The results of the $J-V$ measurements are shown in Fig. 1. We see that adjustment of the *i*-layer thickness between cases (a) and (b) was successful: very similar current densities are obtained for all buffer layer thicknesses. The V_{OC} shows no difference between profiled and nonprofiled buffer design upon changing the buffer thickness. V_{OC} increases from 625 mV (without buffer) to 690 mV using a buffer thickness of about 12 nm.

For the FF we observe a pronounced difference. While the FF increases for an *a*-Si:H buffer layer thickness up to $d(p/i)=d(i/n)=10$ nm, for the normally profiled *a*-SiGe:H-buffer the FF first remains at a low level up to 3 nm buffer layer thickness. Between 3 and 10 nm the FF is nearly 2% (absolute) higher for the *a*-Si:H buffer compared to the normally profiled *a*-SiGe:H buffer. Above 10 nm the FF for the cell structure with the *a*-Si:H buffer finally decreases because of the thicker 1.5 eV *a*-SiGe:H *i* layer necessary to obtain the same j_{SC}. Surprisingly, the band-gap profiling at the p/i and i/n interfaces can be even inverted without any loss in FF and V_{OC}. The performance of such an inversely profiled *a*-SiGe:H buffer [case (c)] is also presented in Fig. 1. In this structure the worst case is realized by applying two band-gap steps, a small band gap (1.5 eV) and an enhanced defect density at both interfaces.

Motivated by these latter results of the inversely profiled *a*-SiGe:H buffers, we investigated how far the position of *a*-Si:H at the beginning (or the end) of the graded *a*-SiGe:H buffer plays a role. This was examined by a very thin *a*-Si:H buffer (of only 3 nm thickness), which is built in at various positions. The distance d between the thin *a*-Si:H buffer and the doped layer at the p/i (i/n) interface was varied, keeping the *a*-Si:H buffer thickness at the i/n (p/i) constant at 9 nm. Figure 2 shows V_{OC} and FF as a function of distance d between the doped and the *a*-Si:H layers. V_{OC} behaves very similar upon variation of distance d at both interfaces. V_{OC} remains unchanged upon a shift of the *a*-Si:H buffer away from the doped layer up to a distance of $d=9$ nm. Above this distance V_{OC} decreases. Already with this thin *a*-Si:H buffer at the interfaces V_{OC} is considerably enhanced compared to no buffer.

For the FF, however, remarkable differences are found for the variation of distance d at the p/i and i/n interfaces, respectively. Without the *a*-Si:H buffer at the p/i interface FF is high. Introducing a thin (3 nm) *a*-Si:H buffer at the interface ($d=0$) already reduces the FF (Fig. 2) and the FF decreases further upon increasing distance d. On the other hand, at the i/n interface without the *a*-Si:H buffer or with an *a*-Si:H buffer directly at the interface ($d=0$) the FF is on a low level (Fig. 2). Surprisingly, the FF increases if the thin *a*-Si:H buffer is shifted away from the n layer. For 3 nm $<d<$6 nm the FF reaches a maximum and decreases again for $d>$6 nm.

It thus appears as if positions d from the interface at which the *a*-SiGe:H solar cell is most susceptible to changes of the buffer layer is different for the p/i and i/n interfaces, respectively. While at the p/i interface FF is already high without an *a*-Si:H buffer [and cannot be further increased by increasing the buffer thickness at the interface (not shown here)], at the i/n interface a position of $d=6$ nm away from the n layer is the most critical position which needs implementation of an *a*-Si:H buffer layer. This is also confirmed in the following where we have replaced the *a*-Si:H buffer of the above experiment (Fig. 2) by an *a*-SiGe:H buffer with a band gap of only 1.4 eV (Fig. 3). Again, distance d between the thin *a*-SiGe:H buffer and the doped layer at the p/i (i/n) interface was varied, keeping the *a*-Si:H buffer thickness at the opposide i/n (p/i) interface constant at 9 nm. In Fig. 3 FF and V_{OC} as a function of distance d between the doped layer and the *a*-SiGe:H layer are shown. Again, V_{OC} behaves similar upon variation of distance d between the doped layer and the thin *a*-SiGe:H buffer on either interface side. For this case V_{OC} exhibits its lowest value for an *a*-SiGe:H buffer located at the interface ($d=0$ nm). Above this distance it recovers again to V_{OC} values obtained without any buffer at the interface.

For the FF, again, remarkable differences are found for the variation of distance d at the p/i and i/n interfaces, respectively. A minimum in the FF is observed using a 3 nm a-SiGe:H buffer layer (1.4 eV) at the p/i interface ($d = 0$ nm). Upon increasing distance d between the p layer and the a-SiGe:H buffer the FF recovers to the value with no buffer at the p/i interface. Again, at a distance $d = 6$ nm from the i/n interface the influence of the buffer is most pronounced, but this time a minimum in the FF is found at this position.

The results show that different designs of the interface region like the simple a-Si:H and normally or inversely profiled a-SiGe:H buffers yield nearly the same performance once the interface layer thickness exceeds a certain value. In particular, V_{OC} and the FF reach the same high level for any of the applied buffers. It can be concluded that band-gap profiling near the interface does not play an important role, a simple a-Si:H buffer is sufficient.

The results obtained with the very thin a-Si:H buffer at various positions near the interface could be the ''key'' structures to explain the experimental results for inverse band-gap profiling. Because there is no beneficial effect of the band-gap profiling itself, it is possible that a-Si:H in the inverse profiled a-SiGe:H buffer at the i/n interface is responsible for the high FF values. This is supported by the results presented in Fig. 2 for the thin a-Si:H buffer.

The results with thin buffer layers in Figs. 2 and 3 show that the solar cell performance (FF and V_{OC}) exhibits a very pronounced dependence on (a) the side (p or n side) where the buffer is located, (b) the position of the buffer layer relative to the doped layers, and (c) the optical band gap of the 3-nm-thick buffer (1.8 or 1.4 eV). It is remarkable in this context that such a big difference in the FF (ΔFF$=12\%$) is observed at a position $d = 6$ nm from the i/n interface using different optical band gaps. While V_{OC} shows the same trends for both the p and n side, the FF has a more complex behavior. The reason for this behavior is not known at this point and should be a challenge for device simulations.

In summary, it was shown that profiled a-SiGe:H buffers as an interface layer in a-SiGe:H solar cells can be replaced by simple a-Si:H buffer layers without any drawbacks in solar cell performance and, surprisingly, an inverse profiled a-SiGe:H buffer works also very well. More insight is gained by a series of test cells with 3-nm-thick buffer layers at various distances from the p/i and i/n interfaces, respectively. These cells show that no buffer is necessary at the p/i interface, while a buffer at the i/n interface is important for solar cell performance. Here, the distance from the i/n interface plays a crucial role and is most effective 6 nm away from the interface (in our case). The difference between the p and n sides mainly shows up in the behavior of the FF, while V_{OC} behaves similarly in both cases. The experiments lead to a critical discussion of the widely used design concepts of band-gap graded p/i and i/n interface layers. This should lead to a revision of these concepts and a deeper understanding of a-SiGe:H solar cells.

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[1] J. Zimmer, H. Stiebig, and H. Wagner, J. Appl. Phys. **84**, 611 (1998).
[2] S. Guha, J. Jang, A. Pawlikiewitz, T. Glatfelder, R. Ross, and S. R. Ovshinsky, Appl. Phys. Lett. **54**, 2330 (1989).
[3] E. Maruyama, A. Terakawa, K. Sayama, K. Ninomiya, H. Tarui, S. Tsuda, S. Nakano, and Y. Kuwano, Proceedings of the 23rd IEEE PV Specialists Conference, Louisville, KY (1993), p. 827.
[4] J. Fölsch, H. Stiebig, F. Finger, B. Rech, D. Lundszien, A. Lambertz, and H. Wagner, Proceedings of the 25th IEEE PV Specialists Conference, Washington, DC (1996), p. 1133.
[5] R. A. C. M. M. van Swaaij, M. Zeman, S. Arnoult, and J. W. Metselaar, Proceedings of the 28th IEEE PV Specialists Conference, Anchorage (2000), p. 869.
[6] Y. Nakata, H. Sannomiya, S. Moriukchi, A. Yokata, Y. Inoue, M. Itoh, and H. Itoh, Mater. Res. Soc. Symp. Proc. **192**, 15 (1990).