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Overview of Surface Passivation Schemes for Thin Film Solar Cells

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***Abstract* — This work provides a rapid overview for the current state of surface passivation layer schemes for thin film solar cells: From its fundamentals to solar cell applications, and their perspective. It provides an overview of important literature and prospect considerations based on simulations.**

***Index Terms* — Photovoltaics, Thin film solar cells, $Cu(In,Ga)Se_2$, Surface passivation, Front, Rear.**

I. Silicon surface passivation by use of a dielectric

The idea to use dielectric layers to reduce recombination at (= "passivate") interfaces stems from silicon (Si) PV. Recombination dynamics at semiconductor interfaces have been described by Shockley, Read, and Hall. Their formalism shows that Si surface passivation layers reduce electronic recombination at the interface by two key methods: (i) Chemical passivation – corresponding to a reduction in interface trap density – and (ii) field effect passivation – resulting from a fixed charge density in the passivation layer that reduces the surface minority or majority charge carrier concentration. In advanced Si solar cell design – e.g. the passivated emitter and rear solar cell (PERC), see Fig. 1 – such passivation layers are combined with micron-sized point openings that serve as electrical contacts, both at the rear and front Si surfaces [1,2].

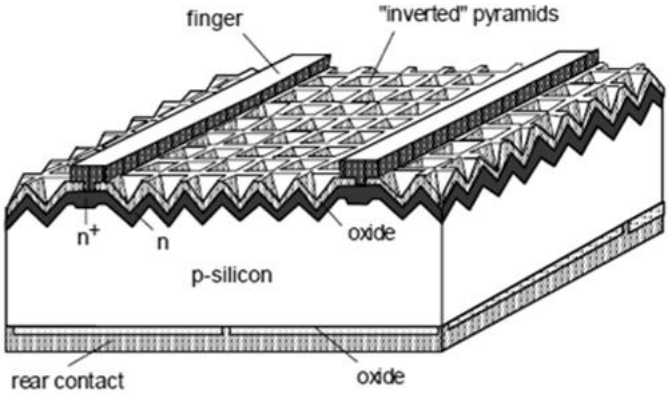

Fig. 1. Drawing of a silicon passivated emitter and rear cell (PERC), which includes SiO_2 front and rear surface passivation layers, taken from [2].

II. Rear surface passivation schemes for CIGS

Various research groups have shown that Al_2O_3 is very suitable to passivate the rear of $Cu(In,Ga)Se_2$ (CIGS) thin film solar cells, which can be explained by a combination of chemical and field effect passivation. Opto-electrical measurements can be used to screen interesting passivation layers, as is shown for Al_2O_3 grown on CIGS [3]. Even more, electrical measurements of similar structures show that the Al_2O_3 layers exhibit a high density of negative fixed charges (its field effect passivation) in combination with a reasonably low interface trap density (its chemical passivation) [4]. In the meanwhile, several groups successfully fabricated Al_2O_3 rear-passivated CIGS solar cells, where recombination at the Al_2O_3/CIGS interface decreased substantially. Uppsala University fabricated rear-passivated solar cells with nano-size point openings generated through the removal of nanosphere-shaped precipitates [5,6], or e-beam lithography [7]; while KIT and ZSW applied photo-lithography [8]. Fig. 2 shows a cross section image of such an Al_2O_3 rear passivated CIGS solar cell.

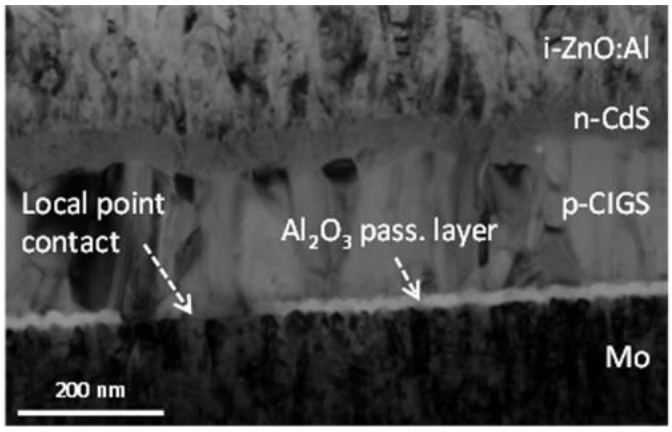

Fig. 2. Transmission electron microscopy cross-section image of an Al_2O_3 rear surface passivated cell with a well-controlled grid of nano-sized local rear point contacts, taken from [7].

Remarkable open circuit voltage (V_{OC}) results have also been achieved for ultra-thin CIGS solar cells with (= despite) a nano-structured SiO_2/CIGS rear interface [9,10], indicating that this SiO_2 layer could be an interesting alternative for Al_2O_3 passivation. M. Schmid has indeed shown reduced

interface recombination at a nanostructured SiO_2/CIGS rear interface [11], very similar to previously acquired results for ultra-thin CIGS solar cells with a nano-structured Al_2O_3/CIGS rear interface [12].

III. Front Surface Passivation Schemes for CIGS

First results indicate that another type of passivation layer will be required to passivate the front of CIGS solar cells. HZB, University of Parma and EMPA have used simulations to show that a positively charged surface passivation layer with nano-sized point openings (e.g. generated as in [13]) would be beneficial to passivate the CIGS/buffer front interface [14,15]. In this case, this positively charged layer causes a n-type inversion layer in the CIGS, which extends the n-type buffer layer, as is shown in Fig. 3. One might even consider to omit the buffer layer completely, and instead use a conformal but ultra-thin (to allow charge carrier tunneling) front surface passivation layer to generate an "inversion layer emitter". This approach is already applied in so-called metal-insulator-semiconductor inversion-layer (MIS/IL) Si solar cells [16]. One surface passivation layer candidate is TiO_2: grown on Si it exhibits a positive charge density [17], and it shows potential for front-passivated CIGS solar cells in [18]. Another candidate is Ga_2O_3: Imec has successfully fabricated Ga_2O_3 front surface passivated CIGS solar cells, a manuscript is in preparation.

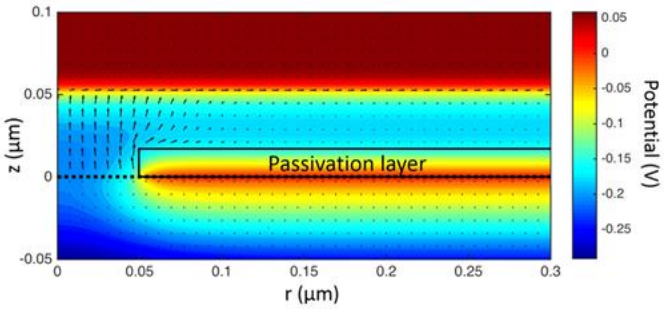

Fig. 3. Simulated potential (color scale) and electron current (arrows) for a front surface passivated CIGS solar cell, by use of a positively charged surface passivation layer, taken from [14]. Note that z = 0 µm corresponds to the CIGS front interface.

IV. Potential of Passivated Emitter and Rear CIGS (PERCIGS)

Integration of front and rear surface passivation layers – combined with approaches for optical confinement [19,20] – into CIGS solar cells with ever thinner absorber layers opens the door for increased cell efficiency, as compared to 'unpassivated' state-of-the-art CIGS solar cells. This is simulated in Fig. 4(a) by use of SCAPS [21], this graph shows solar cell efficiency as a function of CIGS absorber layer thickness for standard CIGS solar cells, and also for an industrially viable and an ideal case of the Passivated *Emitter* (in this case it actually is the Front CIGS interface) and Rear CIGS (PERCIGS) solar cell design (simulation details are mentioned in the figure caption and [4]). Remarkably, for PERC-type Si solar cells a very similar trend in efficiency as a function of Si wafer thickness is seen, as is shown in Fig. 4(b). Note that this trend has been chased by Solexel Inc. who holds the world record for the thinnest Si solar cell: 21.2 % efficiency in case of a 35 µm thick Si 'absorber' layer.

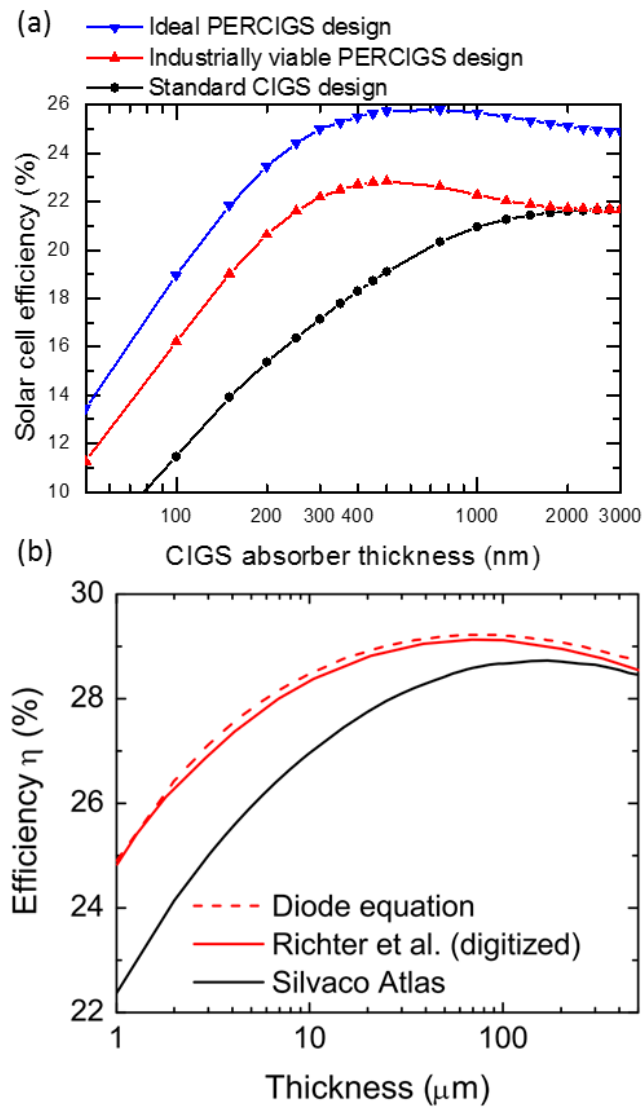

Fig. 4. (a) Solar cell efficiency simulations for state-of-the-art standard CIGS and PERCIGS (with surface passivation, but also light management) solar cells. The standard design contains low rear internal reflection (Mo/CIGS), no surface passivation layers and a high quality CIGS absorber layer (E_{trap} = 0.3 eV). The industrially viable PERCIGS design contains an aluminum rear reflector (Al/Mo/(Al_2O_3/)CIGS rear), surface passivation layers as described in [4], and a high quality CIGS absorber layer. The ideal PERCIGS design contains complete light trapping, surface passivation layers as described in [4], and an excellent quality CIGS absorber layer (E_{trap} = 0.1 eV). (b) A similar graph for Si solar cells, taken from [22].

V. Potential of surface passivation for other thin film

This approach of using dielectric layers to passivate thin film solar cell interfaces is also very valuable for other photovoltaic thin film materials: CdTe surfaces have been successfully passivated by Al_2O_3 films [23,24], and similar passivating layers have been applied for $Cu_2(Zn,Sn)S_4$ (CZTS) [25] and perovskite materials [26,27].

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