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Impact of front-side point contact/passivation geometry on thin-film solar cell performance

Giovanna Sozzi[a,*], Simone Di Napoli[a], Roberto Menozzi[a], Benjamin Bissig[b], Stephan Buecheler[b], Ayodhya N. Tiwari[b]

[a] Department of Engineering and Architecture, University of Parma, Parco Area delle Scienze 181A, 43124 Parma, Italy
[b] Laboratory for Thin Films and Photovoltaics, Empa - Swiss Federal Laboratories for Materials Science and Technology, Ueberlandstrasse 129, CH-8600 Duebendorf, Switzerland

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ABSTRACT

In this work, we perform an extensive campaign of three-dimensional numerical simulations of CIGS solar cell structures to investigate the effect of a surface-passivated CIGS with point contacts openings on the cell performance parameters (J_{sc}, V_{oc}, FF and η). Detailed analysis of the combination of passivation thickness, point contact size and pitch is performed under the hypothesis of highly defective CIGS front surface and ideal chemical passivation: efficiencies close to the case of ideal (i.e., defect-free) CdS/CIGS interface can be achieved by optimized nanometer-scale point contact arrays. To account for field-effect passivation due to positive residual charge density, Q_f, within the passivation layer, we vary Q_f in the range 10^{10}–10^{13} cm^{-2} under the two extreme scenarios of ideal or ineffective chemical passivation. Several examples of CIGS cells with different buffer layers (CdS, ZnO, ZnMgO, In_2S_3, Zn(O, S)) are also analyzed. We find that a positive Q_f in the interval 10^{12}– $5{\cdot}10^{12}$ cm^{-2} can help completely recover the ideal cell efficiency, irrespective of the chemical passivation effect and even in the presence of unfavorable conduction band alignment at the buffer/CIGS heterojunction. This may help devising solutions with buffer materials alternative to CdS, boosting the performance of otherwise surface-limited cells. The effect of grain boundary defect density and position with respect to point contacts is also addressed, with a grain dimension of 750 nm.

1. Introduction

Improvement in conversion efficiency of $Cu(In_{1-x}Ga_x)Se_2$ (CIGS) solar cells has been steady and remarkable, with laboratory-scale CIGS cells reaching efficiencies above 20% on a polyimide substrate [1] and beyond 22% [2,3] on soda-lime glass, thus exceeding those of other thin-film technologies. Improving conversion efficiency is essential to foster the competitiveness of photovoltaics in the energy market, and requires that the main performance-limiting electrical and optical loss mechanisms be identified so that, in a second step, researchers and manufacturers can devise solutions to overcome these limits. Major electrical losses in the cell are non-radiative bulk and interface recombination, which are therefore among the first and foremost performance limiters to take care of.

Record cells [1–3] feature a CdS buffer deposited by chemical bath to ensure suitable interface quality and favorable band-alignment at the CdS/CIGS interface, which results in low recombination rate through the inversion of CIGS surface, so that the cell should be limited by bulk properties, according to [4,5]. The assumption that interface recombination does not play a major role in CIGS solar cells with CdS buffer layer is also supported by several publications discussing the transport mechanism in CIGS solar cells (e.g., [6]). Applying this interpretation to the measured values of the parameters in the one diode model will result in the conclusion that interface recombination is not dominant. However, Scheer showed that interface recombination can be still the dominant mechanism even if the measured activation energy for J_0 is equal or close to the value of the energy band gap of the absorber [7]. Furthermore, the improvements obtained with the recently introduced alkaline post deposition treatment, which affects the interface between CIGS and buffer layer, strongly support the assumption that interface recombination is still limiting the device performance [8].

At the same time the interest in Cd-free buffer layers has been continuously growing, with the twofold purpose of reducing the absorption losses in the short wavelength range caused by the relatively low optical band gap of CdS (2.4 eV), and disposing of toxic Cadmium:

* Corresponding author.
E-mail address: giovanna.sozzi@unipr.it (G. Sozzi).

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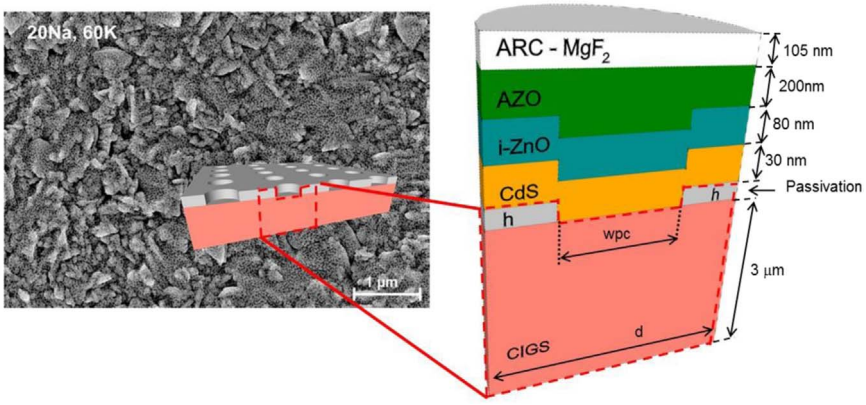

Fig. 1. Left: SEM micrograph of CIGS nano-patterned surface (after [26], supporting information); right: schematic cross-section of the 3D simulated cell.

alternative buffer materials with higher bandgap than CdS are available (the best alternatives being the ZnO-based compounds like Zn(O,S), ZnMgO and ZnSnO and the In_2S_3 [9–12]), but the quality of the interface with CIGS and of electron transport across the hetero-interface are often insufficient to provide efficiencies higher or even comparable with those of CdS-buffer cells [13,14].

Especially in the presence of sub-optimum buffer/absorber interface, the introduction of surface passivation and point contacts might help boost the cell performance, similarly to the case of advanced PERC cells [15] in silicon solar cell technology. Rear-passivated CIGS cells have been proposed with nano-sized point contacts [16], and recently ZnS nano-dots as a passivation film in combination with In_2S_3 point contacts have proven to be a viable strategy to improve the cell performance beyond that of simple planar In_2S_3 buffer by reducing the region of high interface recombination [17]. With the passivation layer approach the requirements of buffer/absorber interface quality can be relaxed, provided that the passivation layer effectively reduces the defective junction and interface recombination losses.

Surface passivation can be used to suppress recombination, whereby the open circuit voltage and the efficiency can be improved. Passivation can lower recombination losses in two ways: i) by reducing the density of active interface defects, impurities or dangling bonds at the CIGS surface (chemical passivation); ii) the presence of charge inside the passivation layer can either repel minority carriers from the semiconductor interface (in the case of negative passivation charge) or enhance surface inversion of the CIGS (in the case of positive passivation charge), thus inhibiting recombination (field-effect passivation) [18]. In the case of silicon technologies, over the years different materials as silicon nitride (SiN), silicon dioxide (SiO_2), amorphous silicon (a-Si), and, more recently, aluminum oxide (Al_2O_3) and hafnium oxide (HfO_2), have proven to possess both chemical and field-effect passivation qualities [19–21].

Among deposition methods, atomic layer deposition, ALD, has the ability to deposit ultrathin layers down to 5 nm, at the same time maintaining good passivation of the surface [19]. The passivation capability of ALD Al_2O_3 is confirmed also when deposited on CIGS [22], probably due to the field-effect more than the reduction of defects at the surface (which is estimated at about 35%) [23]. The control of this field-effect due to charge inside the passivation layer is thus crucial to assure effective surface passivation. Even if the residual charge inside the ALD Al_2O_3 is negative, both its magnitude and polarity can be varied from -3.5×10^{12} cm^{-2} to $+4.0\times10^{12}$ cm^{-2} by inserting additional layers of HfO_2 and SiO_2 [21], making this material an interesting candidate to passivate both the front and rear sides of the absorber, where positive and negative charge, respectively, is optimum for field-effect passivation.

As far as point contact opening is concerned, unfortunately, the conventional patterning techniques used in silicon solar cells are not applicable to chalcopyrite thin films, due to the surface roughness of the polycrystalline absorber and the shorter diffusion length of minority carriers, which requires mean size and distance of localized openings in the nanometer scale [22,24,25]. Recently, though, a novel surface nanopatterning method was presented, obtained by self-assembling of alkali condensates (SALT) [26] forming nanostructures (< 30 nm) on the rough polycrystalline surface of chalcogenide thin films with conformal coverage, thus opening new opportunities for front interface passivation.

The evidence from all these studies suggests the importance of theoretical investigation of the passivation and point contacts geometry to understand their effects on cell performance, with the aim at overcoming the limitations induced by non-optimal interface properties. In this paper therefore we expand on a previous report [27] using three-dimensional (3D) numerical simulations to study the impact of inserting a passivation layer with point contacts at the buffer/CIGS interface. We vary the passivation layer thickness, and the point contact width and pitch, in order to determine the optimum configuration for high efficiency in the presence of highly defective buffer/absorber and passivation/absorber interfaces. The effect of varying the doping of CdS and CIGS in combination with point contacts is also addressed. In this study, we take a closer look at the field-effect passivation induced by the density of fixed charge inside the passivation layer. We mostly focus on a standard CdS/CIGS stack, but results are extended to different buffer materials. Moreover, since the polycrystalline structure of CIGS and the presence of gran boundaries (GBs) are known to influence the cell performance significantly [28,29], although the bulk of this work is focused on single-crystal structures, we also simulate cells featuring surface passivation and contacts openings in the presence of GBs.

The ultimate goal of this work is providing cell manufacturers with guidelines for high-efficiency designs with optimized cross-sectional and layout features, and passivation layer requirements.

2. Materials and methods

Starting from the passivation-plus-local opening geometry achievable by the SALT technique, a picture of which is shown in Fig. 1 (left) (a detailed description of the technique can be found in [26]), we simulated the cell schematically shown in Fig. 1 (right).

The passivation layer thickness h, the point contact width wpc, and pitch d are varied in order to evaluate their effect on cell performance. When h=0, the CdS covers the whole CIGS surface, and the cell structure is the standard one (i.e., with neither passivation nor point contacts).

We modeled the cells using the Synopsys Sentaurus-Tcad suite [30], using cylindrical-symmetry 3D simulations except where otherwise noted. The cell's behavior in the dark is described by the Poisson, electron and hole continuity, and drift-diffusion equations. Recombination via deep defects follows the Shockley – Read – Hall