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ENHANCED CHARGE CARRIER SEPARATION BY POINT CONTACTS IN PASSIVATION LAYERS IN THIN FILM SOLAR CELLS BASED ON HIGH BAND GAP CHALCOPYRITES

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The nonlinear optical I-III-VI_2 material belongs to the chalcopyrite family which is considered to be a promising class of light absorbing material used in 2nd generation thin film photovoltaics. Respective devices with a simple TCO/buffer/Cu(In,Ga)Se_2/Mo/glass structure have already reached power conversion efficiencies, η, close to 20 % [1] on the laboratory scale and 13.4 % on large areas (3459 cm^2) [2]. In contrast to the highly efficient low-band gap Cu(In,Ga)Se_2 chalcopyrite based thin-film solar cells, the photovoltaic performance of the wider band gap $CuInS_2$ and $CuGaSe_2$ chalcopyrite based thin-film solar cells is limited by the recombination at the heterojunction chalcopyrite-window-interface (window layer: transparent conducting oxide (TCO) usually CdS/iZnO/n-ZnO). In principle, the heterojunction should exhibit a high density of defect states at this interface due to lattice mismatch but, nevertheless, the low-band gap cells are dominated by bulk rather than interface recombination which has been explained by a low interface recombination velocity and/or an n-type chalcopyrite surface (inverted surface and buried interface) [3]. In the wider-band gap cells, the band line-up is not directly in favour of an inverted interface and there is a conduction band cliff between the chalcopyrite absorber and the buffer layer (usually CdS). This leads to a reduced barrier for recombination and, consequently, a significantly lower efficiency has been found due to interface recombination. Recent published *jV* curve analysis results of wider-gap $CuInS_2$ and $CuGaSe_2$ solar cells [4, 5] show the limitation of these cells by interface recombination over a reduced barrier. Therefore, it is of high relevance to use an appropriate passivation layer concept in order to decrease the defect states density at the chalcopyrite/window interface.

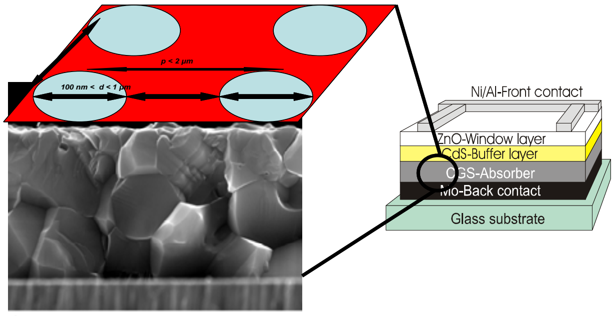

Figure 1: *Point contact model:* The point contacts are embedded in an appropriate passivation layer which is deposited on top of the p-type chalcopyrite surface of the thin film heterojunction device (right). The new heterogeneously constructed passivation layer (red) covering completely the polycrystalline chalcopyrite surface is illustrated schematically on the left hand side. The passivation layer contains a periodic arrangement of point contacts (light blue), while the point contact diameter and the distances between the point contacts are in the range of the diffusion length of the photogenerated charge carriers in p-type chalcopyrite of 1-2 µm.

We proposed here a point-contact geometry at the front side of thin film chalcopyrite solar cell devices which is similar to the concept of contacts at the rear side of high-efficiency silicon based solar cells. While point contacts have previously been used only in high-quality laboratory cells the application of point contacts to industrial solar cells has recently been reached [6]. The concept includes an interfacial defect state passivation and a current transport only through these point contacts that cover a few percent of the device area, while the rest of the surface is electronically passivated by a dielectric coating. In order to reduce the series resistance the contacting area is distributed over the whole device area. Fig.1 shows schematically the concept of point contacts in an appropriate passivation layer which covers completely the chalcopyrite thin film surface and allows a

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current transport of photogenerated charge carriers to the n-type TCO window layer only through these points.

We present here 3D simulations of a novel model based on a conventional TCO-$CuInS_2$-hetero junction solar cell device equipped with point contacts in a passivation layer embedded directly in the p-n hetero junction region by using the WIAS-TeSCA programme [7]. The equipment of such a standard device with electrically conducting point contacts embedded in an appropriate passivation layer such as ZnS shows a highly beneficial effect on the solar cell performance. Especially, the point contact radius, the distance between such points, the interfacial defect density of donor states and the band gap grading in the p-type chalcopyrite have been the relevant parameters of the new model study. Furthermore, we compare our 3D-simulations with 1D-model calculations by using also the SCAPS computer code.

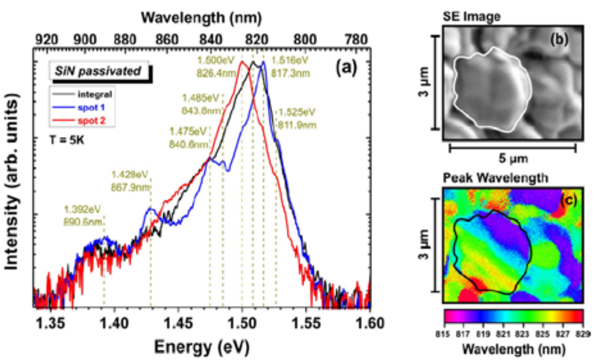

Fig.2: (a) Integral CL spectrum (black) compared to two local spectra taken at different sites of one $CuInS_2$ grain of a Si_xN-passivated thin $CuInS_2$(poly) film. (b) SEM pictures of one grain; (c) CL-peak-to-wavelength picture of the same grain.

Attempts to prepare ultra thin Si_xN passivation layers on $CuInS_2$ surfaces have been successfully performed by means of PECVD. We will present the surface-, interface- and bulk-related electronic defect properties of device-grade uncovered and Si_xN- (Fig.2) and TCO-covered polycrystalline $CuInS_2$ studied by using time- and locally-resolved cathodoluminescence (CL) spectroscopy in a scanning electron microscope at T = 6 K. The focus is set on the electronic defect properties of the blank and TCO- as well as Si_xN-passivated $CuInS_2$ surfaces [8].

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