



Comprehensive simulation model for Cu(In,Ga)(Se,S)₂ solar cells



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ABSTRACT

The modeling of Cu(In,Ga)(Se,S)₂ thin film solar cells enables us to understand device behavior while a reliable simulation with forecasting purpose needs to cover manifold measurement responses. We built up a simulation model to reproduce thermal admittance spectra, capacitance–voltage profiles, quantum efficiency and current–voltage (*I*–*V*) measurements in a broad temperature range from 130 K to 330 K with one parameter set. The comprehensive optical and electrical simulation model has been created as baseline for an indium sulfide buffered Cu(In,Ga)(Se,S)₂ solar cell based on measurement outcome and material characterization. The model ascribes the observed N1 feature ascribing it to a valence band barrier between Cu(In,Ga)(Se,S)₂ and Mo(Se,S)₂ back contact which is also responsible for the roll-over behavior in *I*–*V* measurements. A highly doped p⁺ layer near the heterointerface is accountable for superposition failure of dark and light *I*–*V* curves and kink shape at low temperatures. Two-dimensional simulations further show roll-over dependence on back contact inhomogeneities due to sulfur fluctuations.

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1. Introduction

Among all photovoltaic thin film technologies, chalcopyrite thin film solar cells based on CdS/Cu(In_{1–*x*}Ga_{*x*})Se₂ (CIGSe) heterojunctions demonstrate the highest efficiencies exceeding 20% which competes with the record efficiencies achieved with polysilicon solar cells [1]. Consistent device simulations might assist in further improving the device performance of chalcopyrite solar cells via systematic evaluation of critical parameters (e.g. band gap grading, heterojunction properties). This, however, requires the assessment of relevant material and interface properties (from literature and by experiment), and appropriate implementation of the light propagation throughout the layer sequence (including coherent interaction and scattering of light waves) as well as a reasonable modeling of the transport and recombination characteristics within the entire device. On this basis, accurate device modeling and simulation of particular device characteristics can promote the interpretation of measurement results and could establish a more precise knowledge about internal loss mechanisms as compared to the evaluation of particular measurement results (e.g., by fitting characteristics to analytical models).

Motivated by the complex structure of chalcopyrite solar cells and their non-classical behavior, numerical modeling and simulations have been employed since early days of the research field to correlate particular device and material parameters with the cell output characteristics [2–6]. With appropriate device modeling, many groups reproduced the external quantum efficiency (EQE) spectra and current–voltage (*I*–*V*) response under standard test conditions (STC) [7–10]. Niemegeers *et al.* [11] consistently reproduced both temperature- and illumination-dependent *I*–*V* curves (*I*–*V*–*T*) and temperature-dependent admittance spectra (TAS) with a single model file. However, this device model was not applicable to other studies' measurements [12,13]. Further extensive simulation studies have been conducted by e.g. Eisenbarth *et al.* (*I*–*V*–*T*, TAS) [14] and Decock *et al.* (voltage-dependent TAS) [15]. In addition, more focused simulations address specific issues like intra-band carrier tunneling [16] and grain boundaries [17,18] as well as multivalent [19] and metastable defects [20].

However, a comprehensive device simulation has to employ a device model with a fixed set of material and interface parameters with which various and physically correlated experimental device characteristics can be consistently reproduced. The latter include TAS, *I*–*V*–*T* as well as temperature-dependent external quantum efficiency spectra (EQET) and capacitance–voltage profiles (*C*–*V*–*T*). Despite the progress sketched above, such models have not yet been developed. We aim to close this gap by suggesting a simulation

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model for solar cells based on $\text{Cu}(\text{In}_{1-x}\text{Ga}_x)(\text{Se}_{1-y}\text{S}_y)_2$ (CIGS_{Se}) which consistently reproduces the characteristics TAS, $C-V-T$, EQET and $I-V-T$ with reasonable accuracy. The parameters describing the device model were obtained from detailed characterization of single layers and stacks while crucial input is gained from interpretation of the experimental results obtained from the aforementioned measurements. From simulation and experiment we further provide explanations regarding the interpretation of common features of CIG(S)Se solar cells, namely the heavily debated N1 step commonly observed in TAS spectra as well as the low-temperature distortion of $I-V-T$ curves.

The organization of this paper is as follows. After description of applied samples and experimental methods the results and interpretation of the four main characteristics TAS, $C-V-T$, EQET, and $I-V-T$ are provided in Section 3. After that, the insights obtained from each measurement are discussed in detail and also the device model which is set up from basic material parameters, including band gaps and grading (Section 4). The model refinement comes along with the numerical simulation, thus reproducing of the solar cell characteristics. The doping and defect properties are studied by TAS and $C-V-T$ (Section 4.1). With the knowledge about the optical constants derived from spectroscopic ellipsometry we are able to simulate the EQET (Section 4.2) and finally, $I-V-T$ characteristics (Section 4.3). It should be noted that each model feature that is described to fit in the respective measurement is always cross-checked with the others to find the single model fitting all measurements.

2. Experimental details

The studied CIGS_{Se} samples were processed by AVANCIS GmbH and applied to the sequence $\text{Mo}/\text{Mo}(\text{Se},\text{S})_2/\text{Cu}(\text{In},\text{Ga})(\text{Se},\text{S})_2/\text{In}_x\text{S}_y/\text{i-ZnO}/\text{n-ZnO}$. The polycrystalline CIGS_{Se} absorber was produced by rapid thermal processing of stacked elemental layers in sulfur atmosphere (RTP-SEL) [21,22]. The n-ZnO and i-ZnO, In_xS_y (InS) and Mo films were deposited by conventional physical vapor deposition (sputtering, evaporation). The interfacial $\text{Mo}(\text{Se},\text{S})_2$ (MoSeS) layer is formed reactively with the solid state reaction during the RTP step.

STC- $I-V$ and EQE measurements were performed on 16 CIGS_{Se} samples to verify their common cell performance. For two samples, we conducted TAS, $C-V-T$, EQET, and $I-V-T$ measurements while taking the results of one sample as reference for the simulations. For a more general consideration, we compared these results with those obtained for cells with varied In_xS_y -thickness and for samples with standard CdS buffer (not shown in this work). This further allows clarifying particular issues observed in the TAS and $C-V-T$ spectra. The film thicknesses were quantified with scanning electron microscopy (SEM) performed on device cross sections. The chemical depth profiles used for calculation of the band gap grading were obtained from energy-dispersive X-ray spectroscopy performed on electron-transparent lamellae in a scanning transmission electron microscope (STEM-EDX) [23–25].

TAS and $C-V-T$ were obtained in the temperature range $T=50\text{--}330$ K ($\Delta T=10$ K) from a CryoVac closed-cycle helium contact gas cryostat using a solartron SI-1260 impedance gain/phase analyzer. TAS was measured at zero bias and at $V=-0.3$ V bias, whereas $C-V-T$ was measured with $V=-1.0$ to $+0.2$ V at frequencies of $f=10$ kHz and $f=100$ kHz. For both techniques, an excitation voltage of $V_{ac}=30$ mV was applied. $I-V-T$ measurements were carried out with a cold-finger cryostat (Janis ST-100) in the temperature range $T=100\text{--}330$ K ($\Delta T=10$ K) using a Keithley KTH2400 SMU in four-terminal configuration for data collection. The temperature of the sample was monitored using a Pt-100 temperature sensor mounted on a dummy sample surface. Room-temperature

EQE was measured with a commercial Bentham PVE300 system equipped with an integrating sphere for measurement of the total reflection. EQET was measured with a home-built setup consisting of a cryogenic probe station (Lakeshore TTPX) with optical excitation of the sample by spectrally dispersed illumination from a dual light source (xenon-arc/halogen) transmitted through an optical fiber. The EQET spectra at $T=300$ K were calibrated to the EQE previously measured in the commercial setup at room temperature (RT).

Reliable EQE simulations require an exact knowledge of the optical material properties. Therefore, we performed spectroscopic ellipsometry (SE) on each material with the dielectric functions described in [26]. For SE, we generally used glass substrates covered with the single layer of interest in order to keep the modeling of the dielectric function as simple as possible. For SE measurements on MoSeS, we used glass/Mo/MoSeS/CIGS_{Se} samples and chemically removed the absorber film with aqua regia. Then we measured and modeled the resulting glass/Mo/MoSeS stack to extract the optical constants of MoSeS. With these data, we were able to subsequently characterize the CIGS_{Se} after surface smoothing with aqua regia.

The simulation tool employed for this work was Sentaurus TCAD from Synopsys, Switzerland.

3. Measurement results

3.1. Thermal admittance spectroscopy

In order to investigate the major recombination characteristics, the thermal admittance spectra which give indication of the defect landscape of the CIGS_{Se} layer were obtained first. The detailed interpretation of TAS in the temperature range $T=50\text{--}330$ K and in the frequency band $f=10\text{--}10^6$ Hz gives important input for the device modeling. So, if present, shallow defects can be identified in the space charge region (SCR) of the absorber film since they show up as contributions to the device capacitance.

The individual contributions show up as steps with inflection points f_0 corresponding to the relaxation time of the individual contribution to the device capacitance. In the case of an acceptor state, the observed capacitance step arises from capture and emission of holes from the valence band (VB). Accordingly, the relaxation frequency f_0 is assigned to the thermally activated emission rate ω_0 of the defect [27]:

$$2\pi f_0 = \omega_0 = N_V v_{h,th} \sigma_h e^{-E_a/k_B T} \quad (1)$$

$$N_V v_{h,th} \sigma_h = 2\xi_0 T^2. \quad (2)$$

In Eq. (1), N_V is the effective density of states in the valence band, $v_{h,th}$ is the thermal velocity of holes, σ_h is the capture cross section for holes, and E_a is the activation energy. Eq. (2) pertains to the temperature-dependent dwell time τ of the captured hole in the defect state ($\tau^{-1} = N_V v_{th,h} \sigma_h$) with ξ_0 being a temperature-independent pre-exponential factor. However, admittance steps could have several other origins such as doping relaxation, energy band barriers, or mobility freeze-out. An Arrhenius interpretation according to Eqs. (1) and (2) is than less straightforward. The measured $C-f$ spectra are depicted in Fig. 1 and reveal four temperature-dependent contributions to the device capacitance. The four signatures S1–S4 are partly superimposed which indicates simultaneous response of the involved processes at a given temperature and frequency. Signatures S1–S4 are confirmed in all investigated samples and are thus considered to reflect generic device characteristics whereas slight fluctuations between the samples helped distinguishing the steps from each other.

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