

SUMMARY

The modelling of solar cells enables us to understand the physical phenomena underlying the device behaviour. The use of computer-assisted numerical modelling is convenient for exploring novel solar cell design concepts as well as perform the simulation and analysis of such devices. Numerical modelling is well suited to look deep insight in the details of the physical operation of thin-film solar cells. Till date several modelling tools specific to thin-film PV devices have been developed. Such an approach is beneficial for two primary reasons. First, it is important to know the theoretical parameters towards which, we proceed. This helps to support motivation for the experimental work to be undertaken and gives an accurate gauge of how the work is progressing. Second, realistic, physical device simulations enable for the analysis and possible optimization of experimental devices without the need for physically making the supposed devices. This allows for the crucial saving of resources by performing only the experiments and fabrications that are truly necessary. It is hopeful that this work may serve as a guide to the next series of modelling and simulation efforts that will aid in the development of novel photovoltaic devices and that the analysis performed herein will aid in their experimental realization. A numerical simulation programme, known as Solar Cell Capacitance Simulator (SCAPS) has been used for this purpose.

We have used SCAPS to model and study the behaviour of thin-film solar cells based in different materials such as CdTe, CIGS, SnS and ZnTe. Besides new concepts in photovoltaics such as multilayers solar cells, concentration and intermediate bands have also been covered in this work.

Study of the baseline parameters for the thin-film solar cells discussed in this work was carried out in detail, the comparative analysis for CIGS vs CdTe reveals that CdTe has high open circuit voltage (V_{OC}) and short circuit current (J_{SC}) as compare to CIGS, due to it high band-gap. Conversely, CIGS has better quantum efficiency (QE) then CdTe. ZnTe has high band gap, have high V_{OC} and J_{SC} but its QE is low, but suitable for the concept of intermediate band gap, if inserted, its QE will increase dramatically.

Modern, chalcogenide-based, thin film solar cells based on $CuIn_{(1-x)}Ga_xSe_2$ p-type absorbers are promising candidates for generating pollution-free electricity. CIGS-based devices have bandgaps, which are well suited for absorption of sunlight. Thin-film based on pure Indium, $CuInSe_2$ (CIS) has a band gap of 1.0 eV and that made of pure Ga, $CuGaSe_2$ (CGS) has 1.76 eV, and anyhow substituting Gallium (Ga) for Indium (In) in $Cu(In_x, Ga_{1-x})Se_2$, changes the band gap from 1.0 to 1.76 eV.

The main photovoltaic parameters of a solar cell made of ZnO/CdS/CIGS has been obtained by numerical simulation with SCAPS. For this device we have performed a detailed study of

the effect of Ga content on the overall parameters of solar cells. The obtained results have revealed that the increase of Ga concentration in the absorber layer results in higher efficiency up-to an extent, reaching the maximum efficiency for Ga content about 66%. After optimization of device parameters a maximum efficiency of 30.95 % was reached for 66 % Gallium content. The effect of other layers, ZnO and CdS was also considered, and layers' thicknesses were optimized for better performance. Decreasing of thickness is in favour of good result, but its handling and manufacturing is an issue. The effect of the concentration of donors and acceptors (N_A and N_D) in the CIGS absorber on the overall performance on the cell has been analysed.

The behaviour of ZnO/CdS/CIGS (Ga, 45%) as a function of the concentrated irradiation has also been studied. The conversion efficiency reaches a maximum for about 20 SUN illumination and ranges from 27 % for 1 SUN and 30 % for 20 SUN.

SnS is a promising nontoxic and earth-abundant material suitable for photovoltaic applications. The photovoltaic cell consists of SnS absorber layer, CdS as buffer and ZnO as optical window layer, following the sequence p-SnS/CdS/ZnO. Photovoltaic solar cells based on Tin Sulphide (SnS) absorbers have been analysed by using SCAPS. After optimization of different parameters and layer thicknesses a maximum efficiency of 10.6%, V_{OC} of 0.92 Volts, J_{SC} of 13.4 mA/cm² and Fill Factor of 86.3% were reached. Simulation studies by varying several solar cell parameters such as thickness of various layers reveal that increasing the thickness of absorber layer results in higher efficiency. The concentration of shallow acceptors in the SnS has a crucial effect in the conversion efficiency, which rises up to about 15% for acceptor concentrations of 10¹⁹ cm⁻³. The effect of the compensation ratio between donors and acceptors was also analysed but its effect on conversion efficiency is insignificant.

Solar cells based on II-VI semiconductors are also among the leading candidates for low-cost photovoltaic conversion of solar energy due to their high absorption coefficients and therefore the low material consumption for their production. The analysis of zinc telluride based (ZnTe) thin films solar cells was carried out by using SCAPS. The I-V characteristics, based on dark and illuminated were simulated for the different configuration of input parameters. It has been revealed that increasing the ZnTe thickness (0.5–2.0 μm) results in higher efficiency of PV devices. Parameters such as thickness of various layers reveal that increasing the thickness of absorber layer results in higher efficiency. ZnTe is a p-type semiconductor with a bandgap of about 2.2-2.6 eV, which is too high for an efficient harvesting of solar photons but is suitable for hosting an intermediate band and spread the range of photons absorption.

Intermediate band (IB) is an interesting concept for improving the conversion efficiency of photovoltaic devices and deserves to be studied. Theoretically the maximum conversion efficiency for a PV device based on a single absorber layer is limited by the so called 'Queisser-Schotckly limit'. However, using Intermediate Band materials as absorbers PV devices can

surpass this limit. For such materials efficiencies up to 60 % have been proposed. It is possible to simulate the absorption coefficient of such an IB solar cells and we then use SCAPS for assessing the behaviour and performance of this kind of materials and devices. We have analysed the main PV parameters of a PV solar cell based on ZnTe:O as an absorber layer. The simulation of the structure ZnO/CdS/ZnTe:O solar cell gives an efficiency of 60 %, while the structure ZnO/CdS/ZnTe without IB reaches efficiency below 10 %. The reason for high boosting of QE is the harassment of low energy photons that wasted otherwise. CuGaS₂ has been proposed as a suitable material for hosting an IB by doping with V and Cr (CuGaS₂:V and CuGaS₂:Cr). Theoretical calculations for solar cells based on this IB material predict conversion efficiencies as high as 46.7 %. However, our attempts for modelling such a device did not produce results because SCAPS simulation always failed.

Multi-layer concept will open a new window for researcher, if they boost the performance further. Replacing the existing CIGS by multilayer, and simulated, ZnO/CdS/CuInSe₂/CuGaSe₂ gives very encouraging results of efficiency 30-40 %, with a thinner value of the absorber layer that will further decrease the material use by 35-40 %.