Numerical simulation of thin film solar cells: practical exercises with SCAPS

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Abstract

SCAPS is a numerical device simulator for thin film solar cells, which is freely available to the PV research community. Here two exercises are presented which were used in a training session during the Numos workshop, Gent, March 2007. One exercise is a basic one well suited for starters, and is illustrating the elementary features of the programme. The other exercise makes use of more advanced features like the batch operation, and is intended to users with already a basic experience. At the same time, a clearly non-ideal behaviour of polycrystalline thin film solar cells (here of the CIGS family) is highlighted and illustrated convincingly: a variety of parameters can cause strongly non-ideal I-V curves, showing cross-over, S-shape and even low fill factors $FF < 25\%$.

1. Introduction

This hands-on-session is devoted to the simulation programme SCAPS, developed at the University of Gent [1].

NUMOS participants, new in the field of numerical modelling of thin film solar cells, have been introduced in the basic principles of optical and electrical solar cell modelling by means of tutorials, oral presentations with an introductory and more general character, and by oral and poster presentations with advanced applications and research contributions. In the demonstration part of this session, several optical and electrical simulation packages, including SCAPS, were demonstrated by the developers of the software package themselves, or by experienced users.

In the hands-on-session, two exercises of different levels are proposed to the participants.

•   Exercise 1 is addressed to participants who have a basic knowledge of numerical simulation of solar cells (e.g. acquired during the NUMOS workshop), but have no experience with SCAPS. The purpose of the exercise is to get acquainted with the basic functions of SCAPS: simulation of I-V, C-V, C-f, $QE(\lambda)$ curves, and comparing them with measurements. The focus

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will be on a few (three) parameters and their influence on the basic solar cell properties.

- Exercise 2 is addressed to participants who have finished successfully Exercise 1, or who have been working with SCAPS before. They will familiarize with a new feature of SCAPS (from version 2.6 on): the batch mode, which allows a quick scan of one or a few parameters. The physical focus will be on the shape of the *I-V* curves, and how several parameters can cause a highly non-ideal behaviour of the cell, which is beyond the possibilities of analytical treatment.

The exercises are based on SCAPS version 2.6.1. which will be made available to the PV research community shortly after the workshop. The recent extensions (batch mode, tunnelling) are due to J. Verschraegen of ELIS-UGent [2]. The details of the exercises are worked out below.

2.   Exercise 1: The basics of SCAPS – a simple problem.

The purpose is to get somewhat acquainted with the use of SCAPS, and to get a taste of numerical simulation of an actual thin film solar cell. It is definitely too ambitious to solve real research problems in a two hours workshop on numerical simulation.

Therefore, the participants are provided with 'measurements', which are in fact numerical simulations of a simplified CIGS solar cell. It is simplified, because the cell structure is rather simple (one CIGS absorber layer, a CdS buffer layer and a TCO layer; there is only one recombination mechanism in each layer, and no interface recombination is present; there is no charge in the recombination centres). It is also simplified, because in a real cell all kinds of phenomena can in principle occur, which are not implemented in the simulation programme (e.g. grain boundary and other 2-D and 3-D effects, some tunnelling effects…).

The participants are also provided with a 'baseline' problem definition file. This file is identical to the definition file which produced the 'measurements', but for 3 parameters which were changed: the CdS thickness d_{CdS}, the doping density in the CIGS layer N_{ACIGS}, and the density of recombination centres in the CIGS layer N_{tCIGS}. This greatly reduces the number of parameters which should be varied!

The task is thus as follows:

1.   Open the document `Getting Started.pdf` [3] and read it.
2.   Run SCAPS and load the problem definition file `NUMOS CIGS baseline.def`, with Set Problem $\rightarrow$ Load
3.   Play a little bit around with the basic functions, described in `Getting Started` to familiarise with the SCAPS user interface and functions.

4.   Perform a simulation of *J-V* (dark and light), *C-V* (dark), and *QE*(dark and/or light) curves with the standard settings of the Action Panel.

5.   Display the 'measurement' files

      `Numos Ex 1 light.iv`   (an   *I-V*   measurement   under illumination)

      `Numos Ex 1 dark.iv`   (an *I-V* measurement in dark)

      `Numos Ex 1 dark.cv`   (a *C-V* measurement in dark)

      `Numos Ex 1 dark.qe`   (a *QE*(λ) measurement in dark)

6.   Possibly return to the Action Panel to adapt (restrict or extend) the parameter range (*V*-range or λ-range) to the parameter range of the measurement.

7.   Observe that the simulated curves differ from the measurements, and try to find out which of the parameters d_{CdS}, $N_{A\text{CIGS}}$, and $N_{t\text{CIGS}}$ are the prime cause of the deviation (think first, simulate later).

8.   Vary the parameters d_{CdS}, $N_{A\text{CIGS}}$, and $N_{t\text{CIGS}}$ in the Set Problem/Edit panel in order to obtain a better agreement between simulation and 'measurement'.

3.   The batch feature of SCAPS.

Refer to `Getting Started.pdf` for a basic description of the batch options of SCAPS.

Warning:

•   Don't ask too many parameters at a time: the calculation could be much more time consuming than expected. When you have e.g. 3 nested parameters with each 6 values, you ask for 216 simulations…

•   When it goes wrong, or goes too slow to your taste, or you're realising too late that you were too ambitious, keep the SHIFT-key pressed, until the simulation stops. Your calculations done so far are not lost.

•   Make smart use of the lin/log key at the right hand end of each parameter line. Some parameters really ask for a variation on a log-scale (e.g. doping densities), others for a linear variation (e.g. a thickness).

Operating SCAPS in batch mode will save you much time, when it comes to explore the influence of a few parameters on a simulated measurement, e.g. the *I-V* curves. This will be applied in Exercise 2 below.

4.   Exercise 2: Very kinky *I-V* curves.

Until now (in Exercise 1, e.g.) you have only simulated very honest and respectable *I-V* curves, who almost prudishly follow the prescriptions of the (almost) ideal Shockley theory… But in your research, you certainly have

experienced that real cells behave many times much less honestly: weirdly or kinky are sometimes better words to describe them. In scientific terms, we are speaking about *I-V* curves with *roll-over*, about *cross-over* of the light and dark *I-V* curves, about *S-shaped I-V* curves, fill factors *FF* lower than 25 %, … There is no unique physical cause of this kinky behaviour: many parameters can cause some of the cited features to some extent. The purpose of this Exercise 2 is to illustrate this statement.

The task is as follows:

1. Run SCAPS and load the problem definition file NUMOS Exercise 2.def, with Set Problem → Load. It is derived from our baseline file of Exercise 1, but with several complications:

    o   the deep defects now carry a charge (they are either of the donor or of the acceptor type)

    o   both in the deep bulk states as in the interface states, there is a huge asymmetry in the capture cross sections for electrons and holes, i.e. either $\sigma_n \gg \sigma_p$ or $\sigma_p \gg \sigma_n$.

    o   there can be interface states at the CIGS/CdS interface: their concentration is negligibly low in the NUMOS Exercise 2.def-file, but they are there, and you can give them a substantial value whenever you want.

2. Vary a few parameters using the batch facility, and observe that many parameters can cause really degraded *I-V* curves. Examples are given below (running through all the examples would be very ambitious for a one hour exercise; perhaps restrict yourself to (very) few parameters, and try to understand why the cell behaves as shown by the simulations).

3. <u>Influence of the capture cross sections</u> σ_p and σ_n in the CdS buffer. Note that the defects in the buffer are of the acceptor type, and that they have a huge density $N_t = 10^{18}$ cm^{-3}, exceeding the shallow donor density $N_D = 10^{17}$ cm^{-3}… Both σ_p and σ_n markedly influence the *I-V* curves, that can be kinky at will. See Figure 1, Figure 2, Figure 3.

4. <u>Influence of the conduction band mismatch</u> between CIGS and CdS. When the conduction band mismatch between the CIGS absorber and the CdS buffer is 0.3 eV (as in the standard case of this problem), or lower, the *I-V* curves behave decently. But when it is higher than 0.3 eV (thus $\chi_{CdS} < 4.2$ eV), all kinds of wild behaviour is seen: cross-over, S-shape, *FF* < 25 %,…see Figure 4.

5. <u>Influence of the doping densities</u> of the CIGS absorber and the CdS buffer (extrinsic conditions n^+p or np^+, or intrinsic conditions np). When there are no interface states at the CIGS/CdS interface, there is a large

cross-over, but the *I-V* curves remain decent, both on varying N_{ACIGS} (Figure 5) and on varying N_{DCdS} (Figure 6).

6. <u>Influence of the interface recombination</u>. Extrinsic n^+p or np^+ junctions are rather robust against interface states, or intrinsic *np* junctions are very sensitive. This is seen in Figure 7 where N_{ACIGS} is varied and N_{DCdS} is kept constant, and in   Figure 8 where N_{DCdS} is varied and N_{ACIGS} is kept constant. In Figure 9 the interface states density N_i is varied for a symmetric junction with $N_{DCdS} = N_{ACIGS} = 10^{16}$ cm^{-3}.

7. <u>Influence of the buffer thickness</u>. Exclude interface states, and choose interesting σ_n and σ_p values from the study of item 3 above. Figure 10 is for $\sigma_n = \sigma_p = 10^{-13}$ cm^2.

8. … the study of a thin film solar cell is really open ended, and even a relative simple structure doesn't stop amazing…

The examples below may serve as a guideline, or excite to deeper investigation.

References

[1] M. Burgelman, P. Nollet and S. Degrave, "Modelling polycrystalline semiconductor solar cells", *Thin Solid Films*, **361-362**, 527-532, 2000

[2] J. Verschraegen and M. Burgelman, "Numerical modeling of intra-band tunneling for heterojunction solar cells in scaps", presented at the European Materials Research Society Conference (Symposium O: Thin film chalcogenide photovoltaic materials), E-MRS, Nice, France, may 29 – june 2, 2006. To be published in Thin Solid Films, september 2006.

[3] All files associated with the exercises described here (thus: definition files, measurement files, absorption files; the Getting Started short manual) are made available at the Numos website http://www.elis.ugent.be/numos and/or can be requested from the authors.
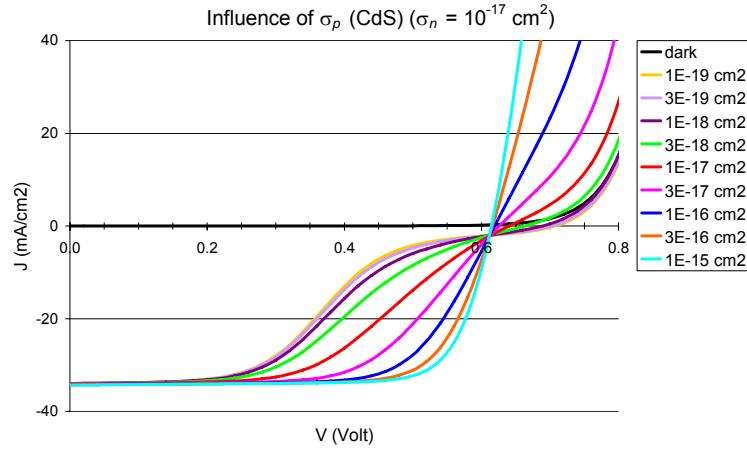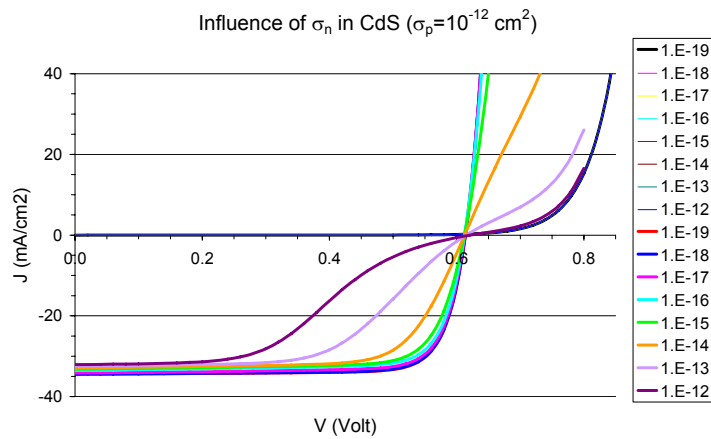
Figure 1   Influence of the capture cross section of the acceptor-type deep states in CdS: $N_t = 10^{18}$ cm^{-3}, $\sigma_n = 10^{-17}$ cm^2, σ_p varying from 10^{-19} cm^2 (worst I-V curve) to 10^{-15} cm^2 (best I-V curve), with 2 curves/decade of σ_p. The dark I-V curve is also shown; it does not depend on the σ_p value.

Figure 2   Influence of the capture cross section of the acceptor-type deep states in CdS: $N_t = 10^{18}$ cm^{-3}, $\sigma_p = 10^{-12}$ cm^2, σ_n varying from 10^{-19} cm^2 (best I-V curve) to 10^{-12} cm^2 (worst I-V curve), with 2 curves/decade of σ_n. The dark I-V curves are also shown; they do not depend on the σ_n value.
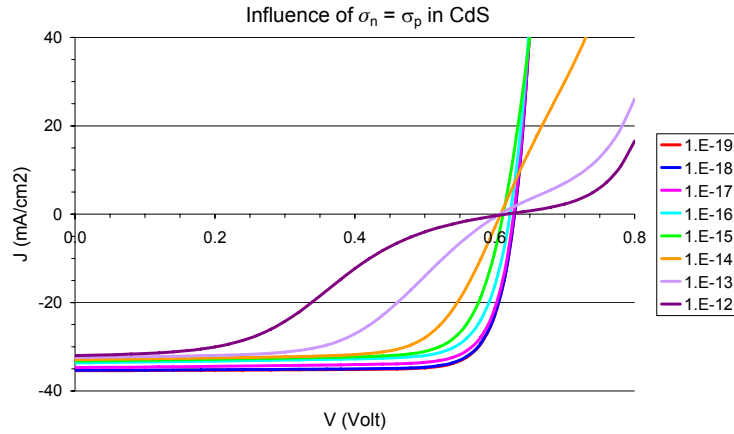
Figure 3   Influence of the capture cross sections of the acceptor-type deep states in CdS, with $N_t = 10^{18}$ cm^{-3}. Now σ_p and σ_n are both varying, but always $\sigma_p = \sigma_n$. The variation is from $\sigma_p = \sigma_n = 10^{-19}$ cm^2 (best *I-V* curve) to $\sigma_p = \sigma_n = 10^{-12}$ cm^2 (worst *I-V* curve). The dark *I-V* curves are not shown; they do not depend on the σ values.
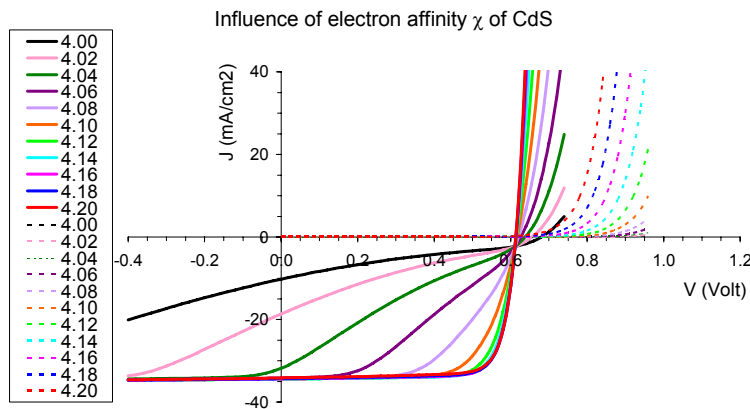

Figure 4   Influence of the electron affinity χ of the CdS buffer: χ varies from $\chi = 4.20$ eV (best *I-V* curve) to $\chi = 4.00$ eV (worst *I-V* curve, *FF* = 0.245!) in steps of $\Delta\chi = 0.02$ eV. In the CIGS absorber is $\chi = 4.50$ eV, and in the ZnO window is $\chi = 4.45$ eV. The illuminated curves (AM1.5G, 1 sun) are in solid lines, the dark curves are in dashed lines with the corresponding colour.

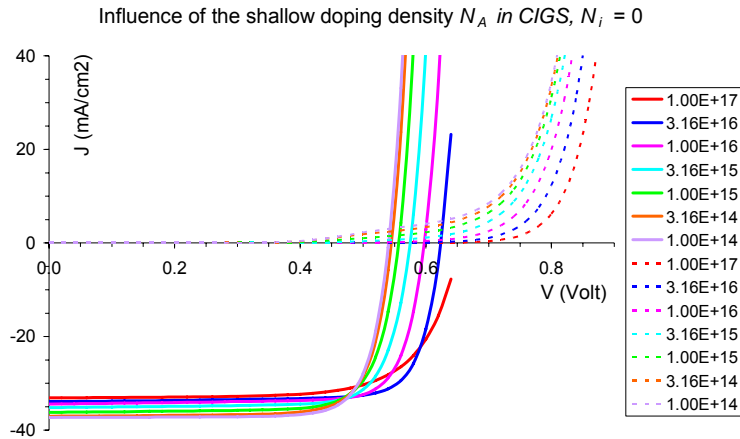Influence of the shallow doping density N_A in CIGS, N_i = 0

Figure 5   Influence of the shallow acceptor density N_A in the CIGS absorber, in the absence of interface states ($N_i = 0$). N_A varies from $N_A = 10^{17}$ cm^{-3} (rightmost *I-V* curve of each set) to $N_A = 10^{14}$ cm^{-3} (leftmost *I-V* curve in each set), with 2 values per decade. The standard setting in the problem file was $N_A = 2 \cdot 10^{16}$ cm^{-3}. The illuminated (solid lines) and dark (dashed lines) curves have a corresponding colour. There is a huge cross-over, but the shape of the *I-V* curves is decent.
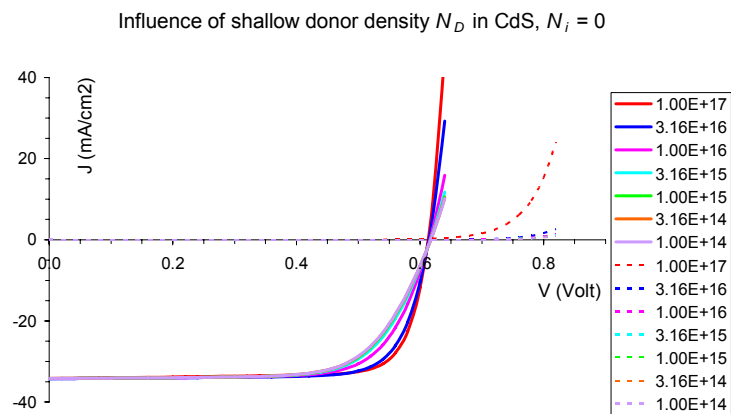
Influence of shallow donor density N_D in CdS, N_i = 0

Figure 6   Influence of the shallow donor density N_D in the CdS buffer, in the absence of interface states ($N_i = 0$). N_D varies from $N_D = 10^{17}$ cm^{-3} (rightmost *I-V* curve of each set) to $N_D = 10^{14}$ cm^{-3} (leftmost *I-V* curve in each set), with 2 values per decade. The standard setting in the problem file was $N_D = 10^{17}$ cm^{-3}. The illuminated (solid lines) and dark (dashed lines) curves have a corresponding colour. There is a huge cross-over, but the shape of the *I-V* curves is decent.
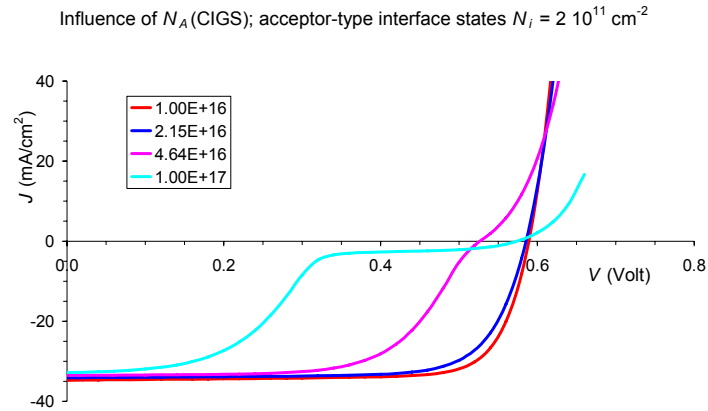
Influence of N_A (CIGS); acceptor-type interface states N_i = 2 10^{11} cm^{-2}

Figure 7   Influence of the shallow acceptor density N_A in the CIGS absorber, in the presence of acceptor-type interface states with N_i = 2 10^{11} cm^{-2}eV^{-1}, uniformly distributed in the gap, and $\sigma_n = \sigma_p = 10^{-14}$ cm^2. N_A varies from $N_A = 10^{16}$ cm^{-3} (best I-V curve) to $N_A = 10^{16}$ cm^{-3} (worst I-V curve), with 3 values per decade. The donor density in CdS was $N_D = 10^{17}$ cm^{-3}. A one-sided n^+p junction is robust against interface states, but a symmetrically doped np junction is almost killed.

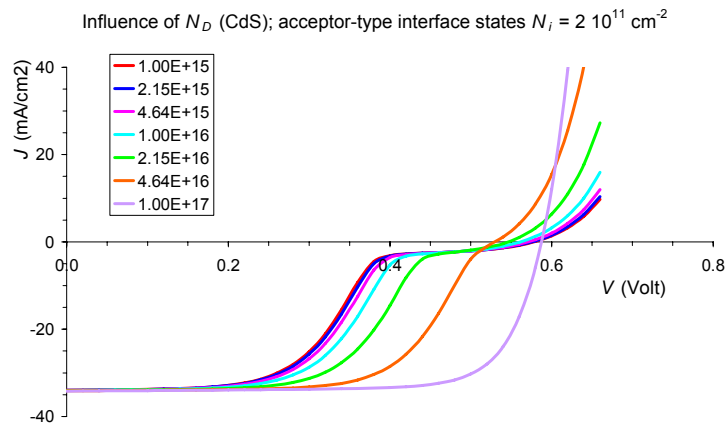Influence of N_D (CdS); acceptor-type interface states N_i = 2 10^{11} cm^{-2}

Figure 8   Influence of the shallow acceptor density N_D in the CdS buffer, in the presence of acceptor-type interface states with N_i = 2 10^{11} cm^{-2}eV^{-1}, uniformly distributed in the gap, and $\sigma_n = \sigma_p = 10^{-14}$ cm^2. N_D varies from $N_D = 10^{17}$ cm^{-3} (best I-V curve) to $N_D = 10^{15}$ cm^{-3} (worst I-V curve), with 3 values per decade. The acceptor density in CIGS was $N_A = 2\ 10^{16}$ cm^{-3}. A one-sided n^+p junction is robust against interface states, but a symmetrically doped np junction is almost killed.

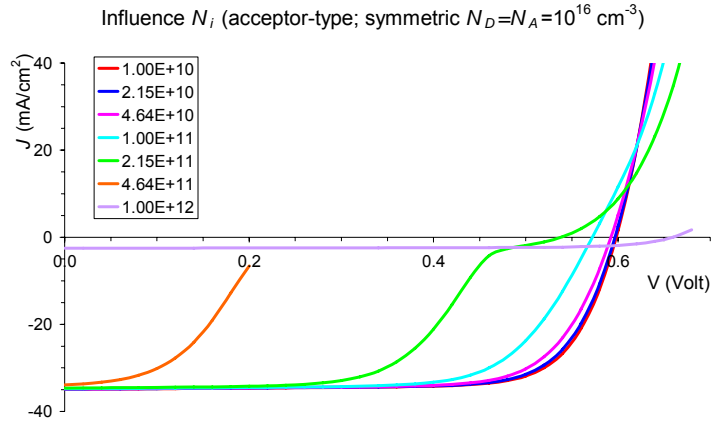Influence N_i (acceptor-type; symmetric $N_D = N_A = 10^{16}$ cm^{-3})

Figure 9   Influence of acceptor-type interface states, uniformly distributed in the gap, and with $\sigma_n = \sigma_p = 10^{-14}$ cm^2, on a symmetrically doped np junction with $N_{ACIGS} = N_{DCdS} = 10^{16}$ cm^{-3}. The interface states density N_i varies from $= 10^{10}$ cm^{-2}eV^{-1} (best I-V curve) to 10^{12} cm^{-2}eV^{-1} (worst I-V curve), with 3 values per decade. Symmetrically doped np junctions are very sensitive to interface states!

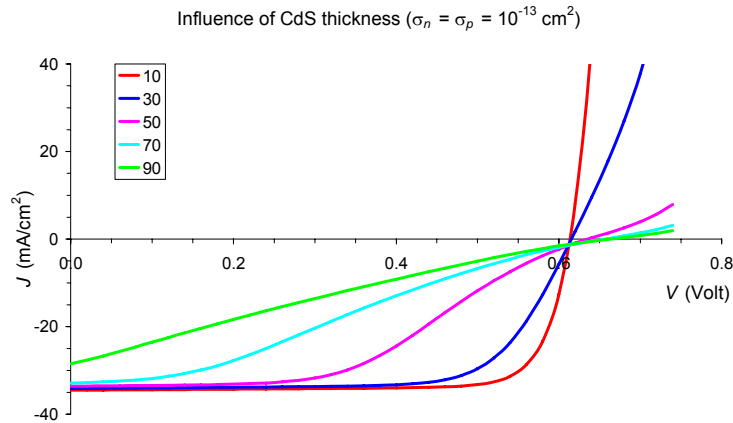Influence of CdS thickness ($\sigma_n = \sigma_p = 10^{-13}$ cm^2)

Figure 10   Influence of the CdS thickness d_{CdS}. There are no interface states. There are acceptor-type deep states in CdS, with $N_t = 10^{18}$ cm^{-3}, and $\sigma_n = \sigma_p = 10^{-13}$ cm^2. The thickness d_{CdS} varies from 10 nm (best I-V curve) to 90 nm (worst I-V curve) in 20 nm steps. The 90 nm curve has $FF = 21.5$ %.