

APPLICATION OF *SC-SIMUL* – NUMERICAL SIMULATION FOR THIN-FILM SILICON BASED DEVICES

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The publicly available device modelling tool *SC-Simul* allows both stationary and time-dependent modelling of a number of experiments with devices like p-i-n or heterojunction diodes. We show applications of *SC-Simul* and model the time-dependent response by studying an amorphous silicon p-i-n diode and voltage switching. For amorphous silicon/crystalline silicon heterodiodes, we study the validity of analytic expressions for the dark current by comparison with numerical results. Modelling results show the significant influence of interface defects in these heterodiodes on the simulated dark current, electroluminescence and electrically-detected magnetic resonance signal.

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1. Introduction

Device modelling is helpful in gaining further insight into the characteristics of devices, because it gives access to internal variables within the device that determine the measurable quantity in an experiment. For example, device design in the electronics industry or simulation of solar cells under different illumination conditions is current practice. Here, applications are presented of the numerical simulation programme *SC-Simul* for versatile modelling of the electronic and optoelectronic properties of semiconductor layers and devices [1], both for stationary and time-dependent modelling of different experiments with user-defined devices.

2. Device modelling

2.1. *SC-Simul* programme description

The programme solves the Poisson equation, the continuity equations for electrons and holes, and the current transport equations including drift, diffusion, and thermionic emission over barriers, if present, in the valence and the conduction band. The programme code in Fortran uses both adapted algorithms and the software library package LSODI for solving these differential equations. More details are given by Rösch [2]. A graphical user interface assists with the modification of device and material parameters and offers first-hand information by graphical representation of the most important output variables like band structure and distributions of currents and recombination rates.

A typical device that has been modelled in some detail is a heterojunction diode of hydrogenated amorphous silicon (a-Si:H) and crystalline silicon (c-Si) [3,4]. Generally, different

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device structures can be designed in *SC-Simul* by a sequence of different semiconductor layers which can be introduced with their specific characteristics. For example, gap states in amorphous silicon are accounted for by introduction of exponential band tails, following Shockley-Read-Hall statistics, and a quasi-continuous distribution of amphoteric dangling bond states, which obey a modified statistics which takes account of the single and double occupancy of dangling bonds. Free charge carriers interact with states in the gap by capture into and emission from these states. From these processes, the recombination rate is calculated. Luminescence is deduced from the local radiative band-to-band recombination rates, thus taking into account the spatial profile of the quasi-Fermi level splitting. From the local radiative recombination rate, the user can process the emitted photon flux, taking into account optical parameters like reflection at the rear surface.

2.2. Modelling of a-Si:H p-i-n diodes and a-Si:H/c-Si heterojunction diodes

A classical device to be modelled is an a-Si:H p-i-n diode. Here, we demonstrate the capability of the programme to model time-dependent processes by studying the time-dependent response after the switching of a p-i-n diode from 0 V to reverse bias.

Another structure to be modelled in some detail here is an a-Si:H/c-Si diode. Of particular importance is a low density of interface defects. This is a technological challenge that is tackled by optimisation of the wafer treatment prior to a-Si:H deposition [5,6] and simulation studies [3,5,7]. A thin defect layer between the amorphous and the crystalline layer is thus introduced, in order to study the influence of interface defects by numerical modelling. The density of defects in this interface layer was varied, in order to obtain different interface defect densities, N_{if} , between $2 \times 10^7 \text{ cm}^{-2}$ and $2 \times 10^{14} \text{ cm}^{-2}$.

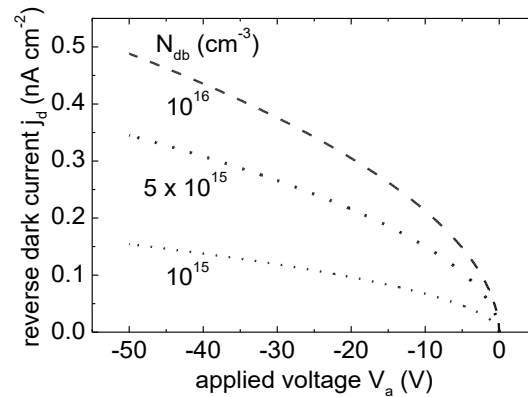


Fig. 1. Steady-state reverse current density for a 19 μm thick a-Si:H p-i-n diode. An increase in dangling bond density results in an increase in the dark current, by enhanced thermal emission.

3. Results and discussion

3.1. Steady-state and time-dependent processes in a-Si:H p-i-n diodes

Fig. 1 shows that the steady-state reverse dark current density of a 19 μm thick a-Si:H p-i-n diode depends to a large degree on the density of dangling bonds N_{db} . The corresponding net-emission rate R_n from dangling bonds is the higher the higher N_{db} (Fig. 2). Also, R_n is increasingly confined to a smaller region of the device for higher N_{db} . Increasing the reverse bias does not change the maximum value of the R_n distribution, but only changes its width (not shown here).

Fig. 3 illustrates the time-dependence of the electric field distribution after switching the diode from 0 V to -40 V. At shorter times, the electric field is almost constant in space. At longer times and in the steady state, however, most of the device is field free. Only in the depletion region with space charge and net emission of electrons and holes does the electric field vary linearly.

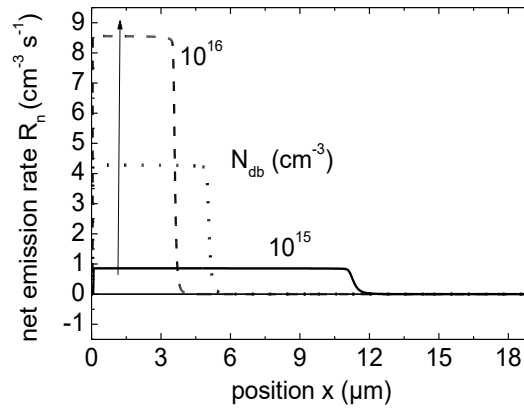


Fig. 2. Net emission rate in steady state for different defect densities.

The results are relevant for sensor applications of thick a-Si:H p-i-n diodes, because of the development of a field-free region unless a very high reverse bias is applied, and for time-of-flight experiments. In the latter, carriers excited by a short light pulse drift through the device. If the experiment is done in steady-state mode with a stationary applied voltage, it is obvious from Fig. 3 that the carriers will not transverse the whole device. Features for the determination of a transit time in the current-time plot will be masked by other effects like deep trapping in the field-free region. This is not unique to a-Si:H p-i-n diodes, because numerical simulations with other material parameters and thick devices show a similar behaviour - namely a spatially inhomogeneous electric field and a field-free region. However, a constant field can be achieved in pulsed-voltage mode for time-of-flight experiments, as the time-dependent simulation shows a spatially constant field at shorter times.

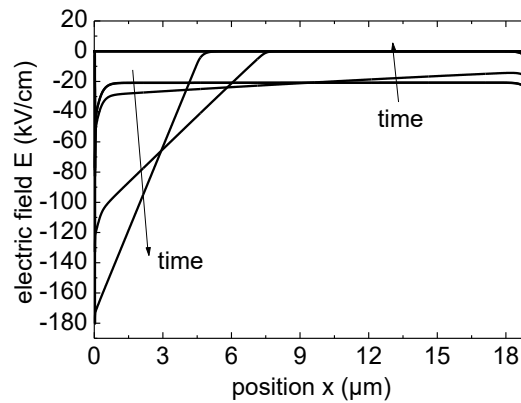


Fig. 3. Time dependence of the electric field after switching a p-i-n diode in the dark from 0 V to -40 V. There is a spatially homogeneous field at short times and a wide field-free region in the steady state.

3.2. Comparison of numerical data with analytic descriptions

Another application for the simulation programme is the comparison of numerical results with analytic formulations, for example in the case of the current-voltage characteristics. Here we show a comparison of calculated forward-bias dark currents for a-Si:H/c-Si heterojunction diodes which have been studied for their electroluminescence properties.

Bresler *et al.* [7] gave an analytical expression for the forward bias dark current density, j_d , which can be rearranged in terms of the Fermi level $E_c - E_f$ in the c-Si, the applied voltage V , and the c-Si diffusion coefficient, D_n , and diffusion length, L_n . For the a-Si:H layer, only the effective

density-of-states, N_{ca} , appears. The Fermi level of the a-Si:H layer has been cancelled out in this expression, given by

$$j_d \approx j_n = \frac{e \cdot D_n}{L_n} N_{ca} e^{-\frac{(E_c - E_f)_{c-Si}}{kT}} e^{\frac{eV}{kT}}. \quad (1)$$

We shall look at the validity of the expression by comparison with numerically modelled current-voltage curves of an (n)a-Si:H/(p)c-Si heterostructure with a 20 nm thick a-Si:H layer, with respect to variation of the doping in the a-Si:H and c-Si layers and the introduction of interface defects in the modelled device.

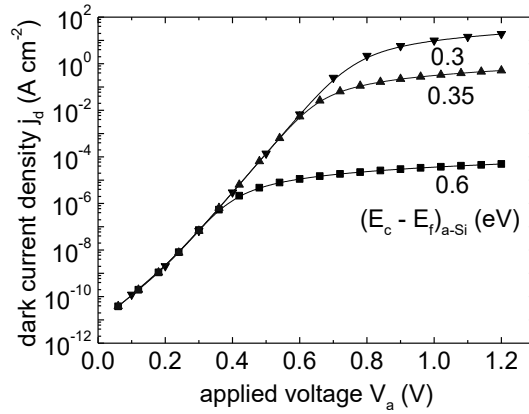


Fig. 4. Steady-state dark current densities vs. forward bias voltage, showing identical values at lower voltages when the Fermi level of the a-Si:H layer is varied. At higher voltages, there are deviations.

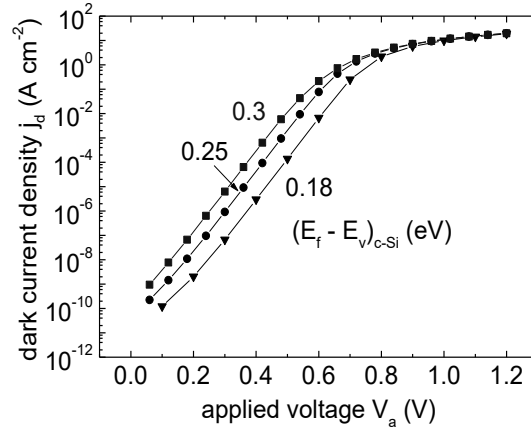


Fig. 5. Steady-state dark current densities vs forward bias voltage, showing a variation with the c-Si Fermi level at lower voltages. At higher voltages, the curves overlap.

Fig. 4 shows the influence of the Fermi level of the a-Si:H layer on the dark current density j_d . As predicted by Eq. (1), j_d does not change with varying Fermi level at lower voltages. At higher voltage, j_d drops strongly if the doping of the a-Si:H layer becomes low. Fig. 5 shows the corresponding variation of $E_c - E_f$ or $E_f - E_v$ in the c-Si layer, with D_n and L_n left unchanged. Again, as predicted by the analytical expression, j_d here varies with the Fermi level as predicted. Also, at a given (lower) V , the j_d values vary exponentially with $E_c - E_f$, as in Eq. (1). The results show that application of the programme allows the determination of limits and validity ranges.

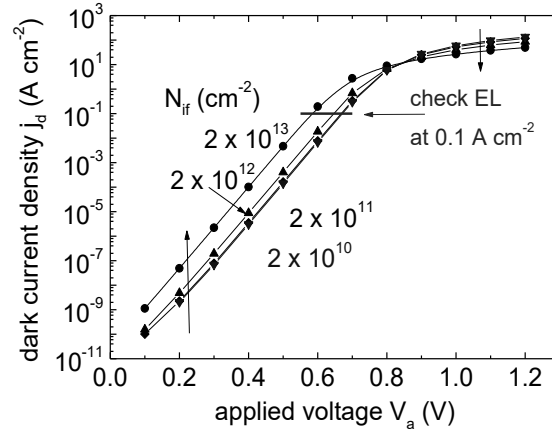


Fig. 6. Influence of interface states on the steady-state dark current densities vs. forward bias voltage. At lower voltages there is an increase in current, while at higher voltages there is a drop in the current with increasing N_{if} .

So far, as also stated by Bresler *et al.* [7] for Eq. (1), interface defects have been neglected. Fig. 6 illustrates that interface defects result in a larger current at smaller voltages and a smaller current at higher voltages. For N_{if} of the order of 10^{12} cm^{-2} , deviations from the low N_{if} results are observed.

3.3. Electroluminescence

A focus of [7] was the study of the electroluminescence (EL) of a-Si:H/c-Si heterodiodes. Thus, we present in Fig. 7 the detrimental effect of N_{if} on the radiative recombination rate R_{bb} at a current density of 100 mA cm^{-2} . The radiative recombination coefficient here was $10^{-14} \text{ cm}^3 \text{ s}^{-1}$ [8]. The results for EL in Fig. 7 show that it is also very important to have a good interface, for example to obtain good photovoltaic properties for these diodes (e.g. [5-7]).

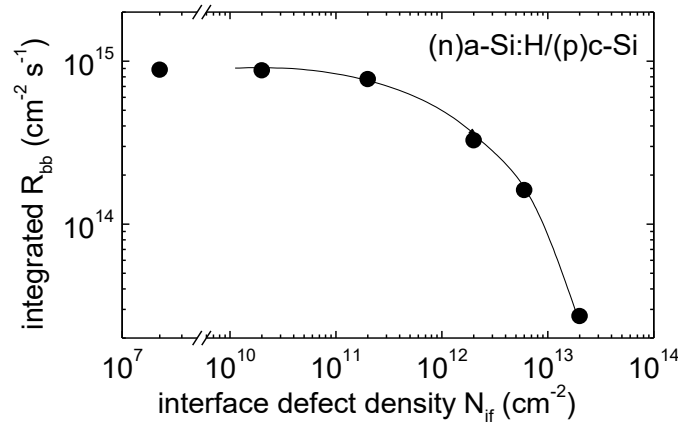


Fig. 7. Decrease in the integrated radiative recombination rate with increasing N_{if} .

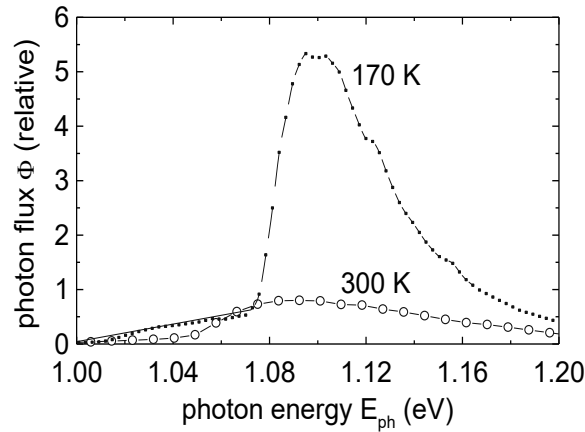


Fig. 8. Calculated electroluminescence spectrum of an a-Si:H/c-Si heterojunction diode at 300 K and 170 K. The spectrum was calculated from the quasi-Fermi level splitting and the absorption coefficient.

It is interesting to note that the EL efficiency, suggested by Bresler *et al.* [7] to be 0.33 % for good diodes, is reproduced by the numerical modelling in Fig. 5 or Fig. 7, if the density of interface defects is small. For the diode of Fig. 7, the efficiency at low N_{if} is about 0.45 %.

With the given spatial distribution of electrons and holes, the EL spectrum can also be calculated [9] from the quasi-Fermi level splitting and spectral distribution of the absorption coefficient. Fig. 8 shows such an example, indicating that the increase in EL is mainly due to an increase in the radiative recombination coefficient with decreasing values of the temperature used in the simulation.

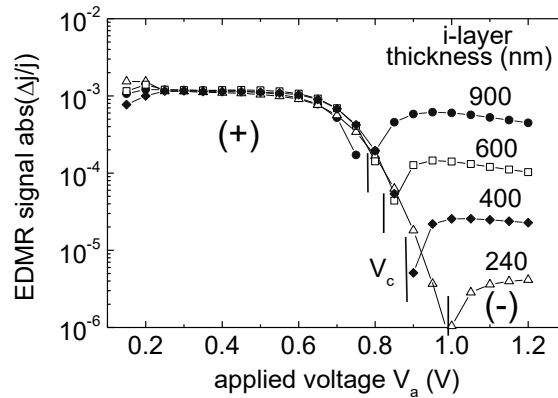


Fig. 9. Modelled EDMR signal for a thickness series of a-Si:H p-i-n diodes. The critical voltages indicate the change-over from enhancing (+) to quenching (-). The absolute value of the quenching signal depends sensitively on the i-layer thickness.

3.4. Electrically-detected magnetic resonance

Electrically-detected magnetic resonance (EDMR) can be modelled by variation of the capture coefficient C_n^0 that describes the spin-dependent capture of electrons into neutral dangling bonds. The free-electron capture rate, $C_n^0 D^0$, where D^0 is the density of neutral dangling bonds, is modified to $C_n^{0*} D^0$ under resonance conditions, with $\Delta C_n^0 / C_n^0 = (C_n^{0*} - C_n^0) / C_n^0 > 0$. The recorded EDMR signal is given by $(j^* - j) / j = \Delta j / j$, where j^* is the current density determined with the increased C_n^{0*} . This approach has been used in the literature [10,11] to model EDMR in a-Si:H and μ c-Si:H p-i-n diodes. Both the so-called enhancing signal with $\Delta j / j > 0$ and the quenching signal with $\Delta j / j < 0$ have been modelled.

Fig. 10 shows an example of the computed EDMR signal for a thickness series of a-Si:H p-i-n diodes. The absolute value shows a dip marked by a vertical line and labelled V_c for the critical voltage. At V_c , the sign of the EDMR signal changes, with (+) indicating enhancing and (-) indicating quenching. The modelled results are in qualitative agreement with [11].

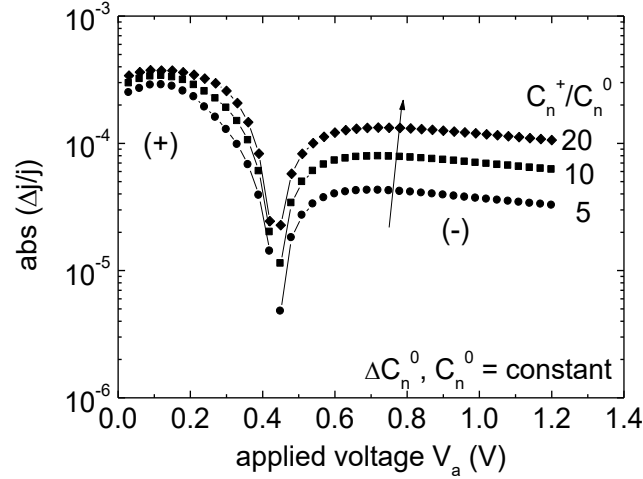


Fig. 10. Variation in the EDMR signal upon variation of C_n^+ . The value C_n^0 for the EDMR sensitive capture transition was kept constant.

Fig. 10 indicates, for a modelled μ c-Si:H diode, that interpretation of the changes in the current density is not always straightforward. The relevant EDMR-related capture coefficient was not varied in the parameter variation, but only the value of the electron capture coefficient for capture into positive dangling bonds C_n^+ , which itself is not EDMR sensitive. The variation in C_n^+ results in a change in the EDMR only because positive dangling bonds are converted to different degrees into neutral dangling bonds. Capture into neutral dangling bonds is EDMR sensitive, and this conversion depends on the C_n^+ value. As for the a-Si:H diodes in Fig. 10, related space charge effects are important to explain the quenching signal. We note that in this case, although the capture coefficient is increased, the result is a decrease in the local recombination rate.

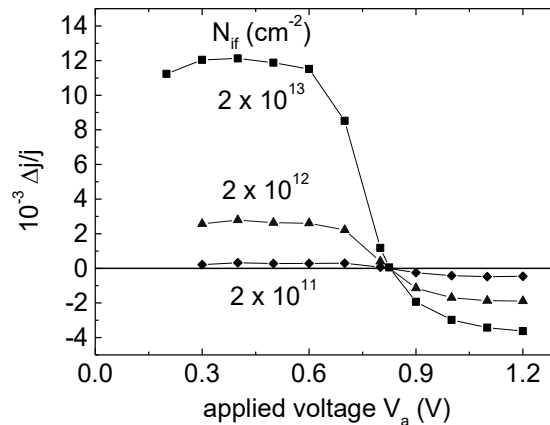


Fig. 11. Variation in the EDMR signal upon variation in interface defect density in an a-Si:H/c-Si diode.

As interface defects have been shown to have a large influence on the EL signal in a-Si:H/c-Si heterostructures, we have looked at the sensitivity of the modelled EDMR spectra to variations in N_{if} . Fig. 11 shows that both the enhancing and the quenching signal vary with N_{if} . The common crossing from a negative to a positive EDMR signal is at the same voltage as for the

current-voltage characteristics in Fig. 6. This indicates the important role of interface defects, which control the current by interface recombination.

The sketched results indicate that via a combination of modelling and experiment, more details on the device physics can be identified in future studies on real devices.

4. Conclusions

Several modelling applications with the simulation programme *SC-Simul* for time-dependent and stationary experiments have been presented. These examples indicate the potential of the programme to contribute to the understanding of the physics of transport, charge distributions and recombination in a variety of devices.

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