DEFECT POOL DENSITY-OF-STATES MODEL IN NUMERICAL MODELLING OF a-Si:H STRUCTURES

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Abstract: Defect pool density-of-states (DP-DOS) model in a-Si:H is presented. The calculation of defect states in a-Si:H based on the defect pool model has been successfully implemented in the ASPIN simulation program. Additionally, variable slopes of band tail states - as a function of doping concentration - have been included in the DP-DOS model. The effect of a leaky Schottky barrier at the front contact on the p-i-n a-Si:H solar cell performance has been analysed. The results of the model with the variable band tail state slopes agree better with the experimental results.

"Defect pool" model gostote stanj pri numeričnem modeliranju amorfnosilicijevih struktur

Ključne besede: polprevodniki, a-Si silicij amorfni, a-Si:H silicij amorfni hidrogeniziran, PIN strukture pozitivno-notranje-negativno, celice sončne, DOS gostota stanj,DP-DOS model gostote stanj "defect pool", gostota stanj, stanja defektna, stanja repov, simulatorji numerični, bariere potencialne, ST-DOS model gostote stanj standardni, DB vezi viseče stanj defektnih

Povzetek: Izračun gostote defektnih stanj znotraj mobilnostne reže, ki temelji na "defect pool" modelu, smo uspešno vključili v ASPIN simulator. Pri izračunu gostote stanj smo upoštevali tudi spremenljiv naklon stanj repov kot funkcijo tipa in koncentracije dopiranja. Obravnavali smo vpliv Schottkyjeve bariere na sprednjem kontaktu na zmogljivost p-i-n amorfnosilicijevih sončnih celic. Rezultati modela s spremenljivim naklonom stanj repov izkazuje boljše ujemanje z eksperimentalnimi rezultati.

1. Introduction

The increasing complexity of heterostructures based on hydrogenated amorphous silicon (a-Si:H) and its alloys demand permanent upgrading of computer models, which are used for their simulation. In contrast to a modelling of monocrystalline devices, in a-Si:H devices one of the key issues is a correct modelling of recombination-generation mechanism and with it connected density of states (DOS) in the mobility gap. States within the mobility gap in a-Si:H can be classified to the valence band tail states, conduction band tail states and between them to the defect states with three possible charges (+, o, -), the so-called dangling bond (DB) defect states. Electrons or holes can be trapped or recombined in these states and the charged states contribute to the space charge affecting the device electrical properties.

Most existing simulation models use for a-Si:H a standard DOS model (ST-DOS) /1/, in which DB defect states are modelled by Gaussian-shaped $D^{+/o}$ and $D^{o/-}$ states placed near the midgap and separated by the effective correlation energy U_{eff}, which was experimentally measured to be positive (Fig. 1). The density of DB states are taken to be constant in the individual layers of the multi-layer a-Si:H structure.

The ST-DOS model (as seen in Fig. 1) leads to positively charged defects in p-type amorphous silicon having a lower energy than negatively charged defects in n-type amorphous silicon, since the U_{eff} is positive. But this energetic position of charged defect states in doped

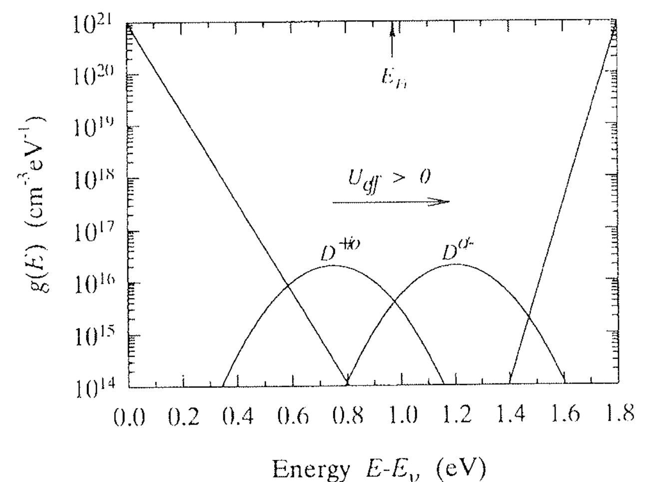

Fig. 1 One-electron density of states distribution according to the standard model (E_F indicated by an arrow).

a-Si:H is not consistent with results found in many experiments /2,3,4/.

A recent theory of defect formation in a-Si:H based on weak-bond dangling-bond reaction determined by a chemical equilibrium process explains most of the a-Si:H behaviour and it is known as the defect pool (DP) concept /5,6,7/. We have implemented this concept into

our simulator ASPIN /8,9/ and the results of this implementation are presented and discussed.

2. Defect pool model and its properties

Thermodynamic approach of defect formation is based on a chemical equilibrium reaction between silicon weak *Si-Si* bonds (the exponential valence band tail) and dangling bonds. In reaction *i* hydrogen atoms can be involved, where *i*= 0, 1, 2 /6/. This approach also postulates a possible distribution of available dangling bond energies due to the inherent disorder of the amorphous network. This is the so-called defect pool, which is assumed to be Gaussian-shaped and centered at the defect pool position E_P. For a sufficiently wide pool, the model leads to negatively charged defects in n-type a-Si:H having a lower energy than positively charged defects in p-type a-Si:H, even when the correlation energy is positive, a previously puzzling result found in many experiments /2,3,4/. The inclusion of the occupancy statistics predicts the formation of three different defect states regarding their charge state and position in the mobility gap. Furthermore, the density of charged dangling bond defects (D^- and D^+) is in thermal equilibrium higher than density of neutral defects (D^0) even in undoped a-Si:H /6/. The equilibrium density of DB defect states depends on the Fermi energy, which leads to a higher density of dangling bonds in doped a-Si:H than undoped a-Si:H.

Our numerical defect pool DOS (DP-DOS) model consists of a standard tail of donor-like states above the valence band edge, a standard tail of acceptor-like states below the conduction band edge, and three Gaussian-shaped DB defect state densities D_n, D_i, D_p, whose density depends on the Fermi energy level E_F according to the derived analytical dependencies, which are in good agreement with measured results /10/. Each Gaussian-shaped DB defect state density is approximated with an exponential dependence on E_F (for values see Table 1) as:

$$g_{D_n}(E,E_F) = gM_{D_n} \cdot e^{-\frac{(E-E_{Dn})^2}{2\sigma_p^2}} \cdot e^{\frac{E_{Fi}-E_F}{kT_n}} \quad (1)$$

$$g_{D_i}(E,E_F) = gM_{D_i} \cdot e^{-\frac{(E-E_{Di})^2}{2\sigma_p^2}} \cdot e^{\frac{E_{Fi}-E_F}{kT_i}} \quad (2)$$

$$g_{D_p}(E,E_F) = gM_{D_p} \cdot e^{-\frac{(E-E_{Dp})^2}{2\sigma_p^2}} \cdot e^{-\frac{E_{Fi}-E_F}{kT_p}} \quad (3)$$

Taking into account a positive correlation energy for doubly occupied state, each dangling bond defect state (D_n, D_i, D_p) is divided into two further peaks (+/0, 0/-), since each defect state can be occupied by zero (+), one (0) or two electrons (-) (Fig. 1). Thus, we can duplicate Eqs. 1-3 for six Gaussian-shaped DB defect states with their peaks at:

$$E_{D_n^{+/0}} = E_p - \frac{2\sigma_p^2}{E_{0v}} \qquad E_{D_n^{0/-}} = E_p - \frac{2\sigma_p^2}{E_{0v}} + U_{eff} \quad (4)$$

$$E_{D_i^{+/0}} = E_p - \frac{\sigma_p^2}{E_{0v}} \qquad E_{D_i^{0/-}} = E_p - \frac{\sigma_p^2}{E_{0v}} + U_{eff} \quad (5)$$

$$E_{D_p^{+/0}} = E_p \qquad E_{D_p^{0/-}} = E_p + U_{eff} \quad (6)$$

In thermal equilibrium, the D_n, D_i, D_p states correspond to doubly occupied (D^-), singly occupied (D^0) and un-

Table 1: Defect pool DOS model input parameters

Parameter	p	i	n
Tail States Parameters:			
Density at E_c, E_v (cm^{-3}eV^{-1})	2.10^{21}	2.10^{21}	2.10^{21}
E_{v0} (meV)	50/90	50	50/80
E_{c0} (meV)	25/45	25	25/40
$\sigma_C v_{th}$ (cm^3/s)	5.10^{-11}	5.10^{-11}	5.10^{-11}
$\sigma_N v_{th}$ (cm^3/s)	5.10^{-9}	5.10^{-9}	5.10^{-9}
Defect States Parameters:			
Concentration (cm^{-3})	10^{18}	10^{16}	10^{18}
U_{eff} (eV)	+0.2	+0.2	+0.2
E_p-E_v (eV)	1.2	1.2	1.2
σ_p (eV)	0.125	0.125	0.125
$\sigma_C v_{th}$ (cm^3/s)	5.10^{-11}	5.10^{-11}	5.10^{-11}
$\sigma_N v_{th}$ (cm^3/s)	5.10^{-9}	5.10^{-9}	5.10^{-9}

	D_n	D_i	D_p
gM_D (cm^{-3}eV^{-1})	2.10^{16}	4.10^{15}	2.10^{16}
$E_D^{+/0}$-E_v (eV)	0.55	0.85	1.20
U_{eff} (eV)	+0.2	+0.2	+0.2
σ_p (eV)	0.125	0.125	0.125
kT (eV)	0.103	10^{12}	0.107

occupied (D^+) dangling bond defect states, respectively.

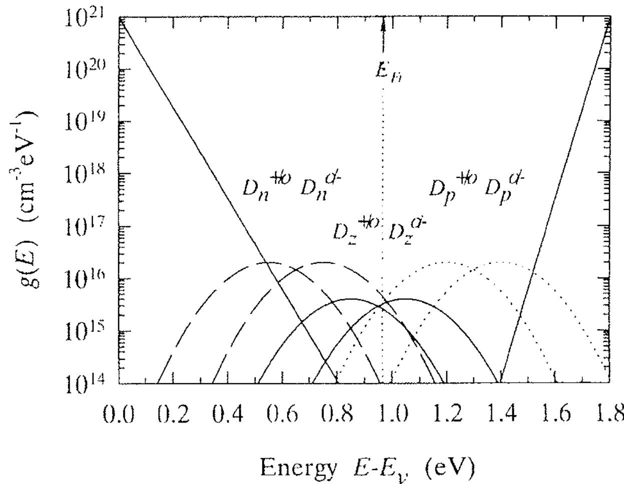

Fig. 2: One-electron density of states distribution according to the defect pool model for intrinsic a-Si:H in thermal equilibrium (E_F indicated by an arrow).

Since the defect pool model implies that the position of the Fermi energy determines the defect distribution, in the p-i-n structure the spatial-dependent defect states density is calculated self consistently from the Poisson's and continuity equations at the equilibration temperature T* (500 K) together with the derived analytical dependencies on E_F (see Eqs. 1-3).

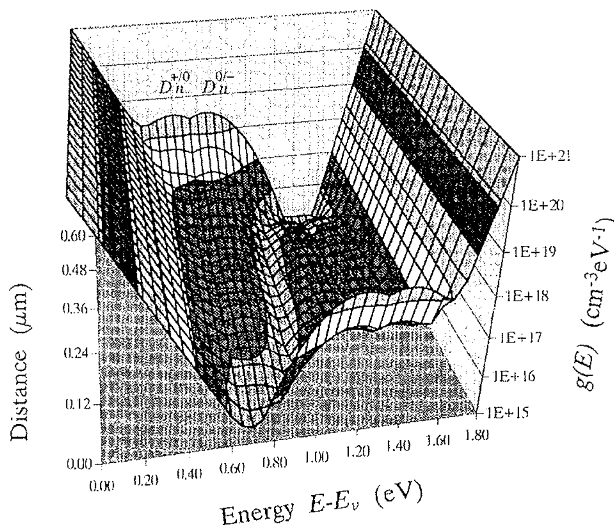

Fig. 3: One-electron density of states throughout the p-i-n structure - calculated from the defect pool model.

The "frozen" gap states distribution profile (Figs. 3, 4) is used to calculate the behaviour of the device at the operational temperature. Out of thermal equilibrium, the charge state of defects becomes a function of the electron and hole concentration.

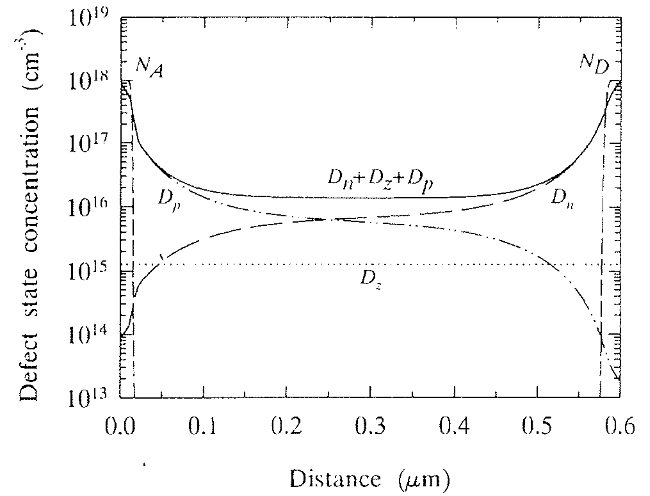

Fig. 4: Defect pool in the p-i-n structure: calculated distribution of defects D_n, D_i, D_p and the doping profile.

3. Results

A lot of scientific attention has been paid to a leaky Schottky barrier at the TCO/p interface /11,12/. Using defect pool DOS model we have analysed how the barrier affects the solar cell performance. Results under AM 1.5 illumination are seen in Fig. 5 (full line). Surface potential barrier V_B ranges from 0.0 V, i.e. the thermal equilibrium value as in the bulk of the p layer, to 0.24 V. Bigger potential barrier increases the diffusion of electrons into the front contact and thus decreasing the J_{SC}. Bigger barrier affects most strongly the V_{OC}. Consequently, the efficiency drops significantly with increasing the barrier.

Recent CPM measurements /13,14/ revealed that the slopes of the band tail states (E_{V0}, E_{C0}) are affected by the doping concentration, especially by boron atoms in a p layer. Based on experimental results, we included a linear fit of this dependence to the DP-DOS model (DP*-DOS) and it is seen in Fig. 6.

The effects of the improved DP*-DOS model on the cell performance are presented in Fig. 5 (dashed line). The J_{SC} is surprisingly bigger. Fig. 7 reveals the difference in the built-in electric field, which is at the bias of 0.0 V in case of variable slopes slightly lower in the i layer, but higher near the surface of the p layer, so that it mitigates the harmful diffusion of electrons into the front contact and improves the collection efficiency in the short wavelength region. Consequently, the J_{SC} increases. On the other hand, the increased tail states in the doped layers contribute to an increase of the recombination rate and thus reducing V_{OC} and FF. In DP*-DOS model, the V_{OC} and FF values seem to be in better agreement with experimental results.

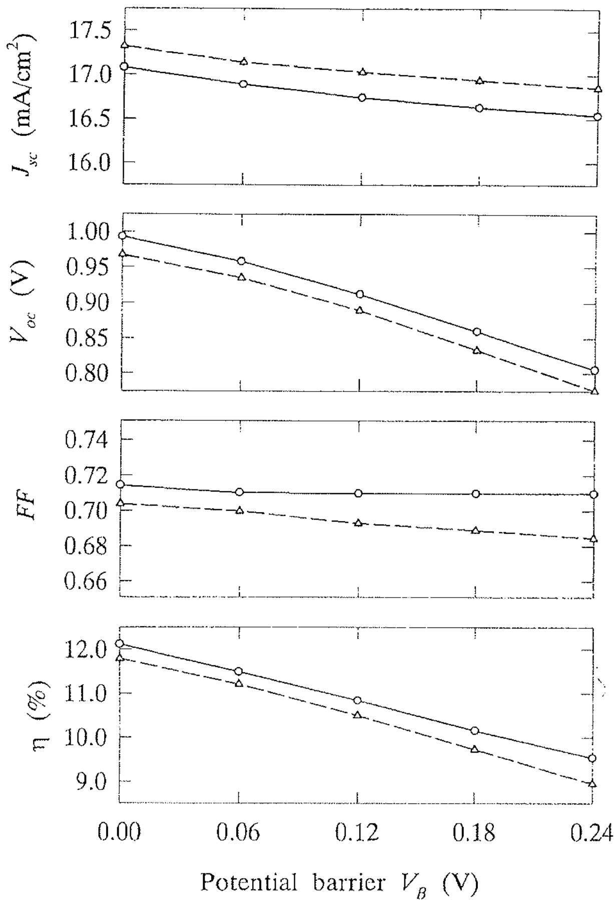

Fig. 5: Photoelectric properties of a p-i-n a-Si:H solar cell as a function of potential barrier at the TCO/p contact interface (full line - constant band tail state slopes; dashed line - variable band tail state slopes).

Another inspection tool is the dark current-voltage characteristic. In Fig. 8 we can see the difference in calculated characteristics for DP-DOS model and DP*-DOS model with the barrier of 0.0 V and 0.12 V. The main difference occurs at applied voltages above 0.5 V, where in case of variable band tail slopes the electric field in the p and i layer drops with applied voltage faster

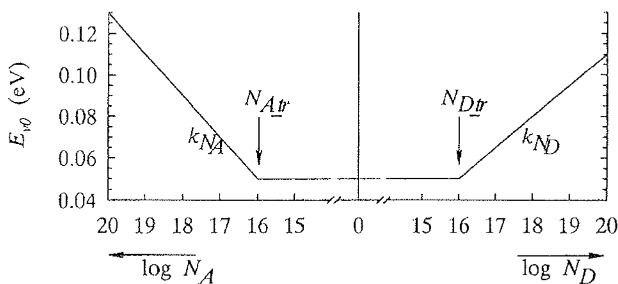

Fig. 6: A model of E_{V0} dependency on doping concentration. Similar dependency holds also for E_{C0} - only initial value E_{C00} is smaller (25 meV).

and the recombination rate in the p layer increases strongly.

The electric field profile in dark calculated from a defect pool DOS models differs significantly from a profile using a ST-DOS model. However, under AM1.5 illumination both approaches give similar profiles. This phenomenon leads to the conclusion that - assuming the DP-DOS models are correct and more exact - the electric field profile is very sensitive to the illumination intensity. By measuring collection efficiency under different

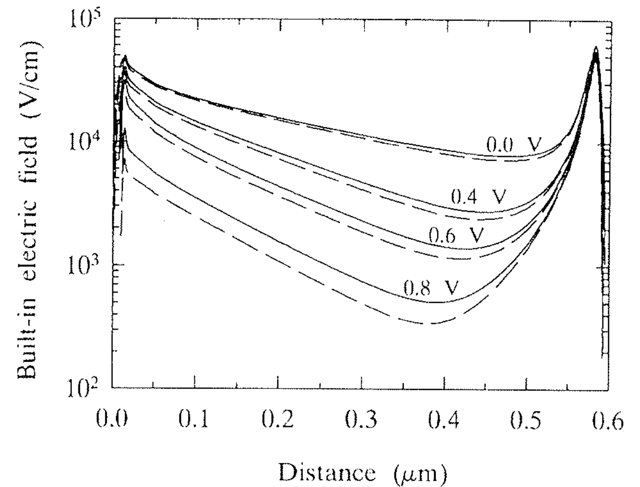

Fig. 7: Calculated electric field profiles under AM1.5 for the surface potential of 0.12 V using DP-DOS model with constant (full line) and DP-DOS model with variable band tail slope (dashed line).

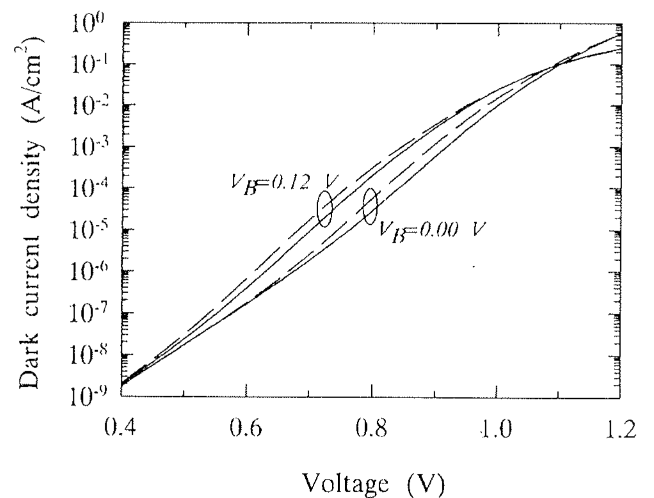

Fig. 8: Calculated dark current-voltage characteristics for DP-DOS model with constant (full lines) and with variable band tail slope (dashed lines) throughout the structure for two surface potential barrier values.

intensities and accompanied with numerical simulations, this could be verified.

4. Conclusions

According to the defect pool concept, we have formed a numerical defect pool model and successfully implemented the calculation of the defect state distribution in the device simulator ASPIN. The possibility of varying the slopes of band tail states as a function of doping concentration has been added. Based on experimental results from literature, a model for variable slopes was proposed. For both, constant and variable slope cases, the validity of the defect pool model for modelling a-Si:H devices was verified for p-i-n solar cells. The model with the variable slopes of band tail states exhibits better agreement with the experimental results and it is certainly more realistic. However, further work, predominantly experimental is necessary to obtain better fit for band tail slope dependence on doping concentration.

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