ELSEVIER

Solar Energy Materials & Solar Cells 65 (2001) 149–155

Solar Energy Materials & Solar Cells

www.elsevier.com/locate/solmat

Improvements in numerical modelling of highly injected crystalline silicon solar cells

Pietro P. Altermatt[a,*], Ronald A. Sinton[b], Gernot Heiser[c,a]

[a] *University of New South Wales, Centre for Photovoltaic Engineering, Sydney 2052, Australia*

[b] *Sinton Consulting, 1132 Green Circle, Boulder, CO 80303, USA*

[c] *University of NSW, School of Computer Science and Engineering, Sydney 2052, Australia*

Abstract

We numerically model crystalline silicon concentrator cells with the inclusion of band gap narrowing (BGN) caused by injected free carriers. In previous studies, the revised room-temperature value of the intrinsic carrier density, $n_i = 1.00 \times 10^{10}\,cm^{-3}$, was inconsistent with the other material parameters of highly injected silicon. In this paper, we show that high-injection experiments can be described consistently with the revised value of n_i if free-carrier induced BGN is included, and that such BGN is an important effect in silicon concentrator cells. The new model presented here significantly improves the ability to model highly injected silicon cells with a high level of precision. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Computer modelling; Band-gap narrowing; c-Si solar cell

1. The experiment of Sinton and Swanson

The value of the ambipolar Auger coefficient, $C_a = 1.66 \times 10^{-30}\,cm^6/s$, is commonly used in calculations of highly injected crystalline silicon solar cells. This value was determined by Sinton and Swanson in 1987 [1] to an uncertainty of 15%, and lies within the error bars of other frequently used values of C_a [2–5]. Sinton and Swanson measured both the steady state and the transient open-circuit voltage of a solar cell. This cell was specially designed so that its losses were dominated by Auger recombination [1]. C_a was obtained by reproducing both measurements with an analytical model, where only C_a needed to be varied because all the other relevant input parameters were known from independent measurements.

* Corresponding author.

PII: S0927-0248(00)00089-1

2. Revisions of silicon material parameters

After Sinton and Swanson's experiment, an important input parameter of the above-mentioned analytical model underwent revision. Green and Sproul [6,7] lowered the most precisely measured value of the intrinsic carrier density of silicon, n_i, from 1.45×10^{10} to $1.00 \times 10^{10}\,\mathrm{cm}^{-3}$ (at $T = 300\,\mathrm{K}$). This affects the extracted value of C_a strongly: lowering n_i increases the modelled open-circuit voltage V_{oc}, and hence C_a has to be increased in order to reproduce the measured V_{oc} values. However, using the revised n_i, the analytical model of Sinton and Swanson yields two C_a values that are significantly different when extracted from the stready state and from the transient experiment, because the former evaluation depends on n_i^2 and the latter on n_i^3, respectively. Thus, Banghart et al. [8] suggested that the high density of induced carriers in Sinton and Swanson's experiment (up to $2 \times 10^{17}\,\mathrm{cm}^{-3}$) may cause free-carrier induced band gap narrowing (BGN). This implies that, in Sinton and Swanson's analytical theory, the old value of n_i was not the intrinsic, but actually the *effective* intrinsic carrier density $n_{i,eff}$, which is larger than n_i due to gap shrinkage, ΔE_g:

$$n_{i,\mathrm{eff}} = n_i \exp \frac{\Delta E_g}{2kT}, \tag{1}$$

where T is the absolute temperature, and k is Boltzmann's constant. However, the parameter-set of Banghart et al. [8] was inconsistent and disagreed with experimental findings. Only after measurements of transport parameters in highly injected silicon [9], and after improvements in BGN theory [10] did Banghart and Gray [11] find a parameter-set to calculate the transient V_{oc} measurements of Sinton and Swanson [1] with a reasonably high level of precision, using the revised n_i and free-carrier induced BGN. Banghart and Gray's results strongly suggest that free-carrier induced BGN influences $n_{i,eff}$ significantly at injection levels generated in C_a measurements. One may think that it is more straight-forward to determine C_a with devices that have no pn junction, so that $n_{i,eff}$ does not enter the data evaluation. For example, a number of authors measured C_a in samples by excess-carrier lifetime measurements of intrinsic silicon [2–5]. However, the Auger recombination rate depends cubically on the carrier density. Hence, experiments without pn junction need very accurate measurements of the photo-conductance, accurate knowledge of the carrier mobility in high-injection conditions, and good models for the evaluation of carrier density profiles during the experiment. In contrast, the pn junction experiments using open-circuited devices need no such knowledge, but mix BGN and C_a.

The experiment of Sinton and Swanson is very valuable for demonstrating consistency between n_i, BGN and C_a. These three parameters form the foundation for the modelling of highly injected silicon solar cells. Such consistency is difficult to achieve because BGN and C_a reflect many-body effects, and hence depend on injection density [5,12]. Above all, we are not aware of a publication reporting on a systematic experimental study of free-carrier induced BGN at room temperature. Neugroschel et al. [13] attempted to extract free-carrier induced BGN from the current–voltage (*I–V*) curve of a highly injected transistor. However, their result was imprecise for a number of reasons: they used the old n_i, they neglected series resistance effects, they assumed that BGN is zero at a carrier density of $1\times10^{16}\,cm^{-3}$, and they extracted the carrier density with a procedure that leads to over-estimated values. Our simulations of their experiment revealed that their *I–V* curve was severely affected by Auger recombination. Thus, larger difficulties were experienced in separating n_i, BGN and C_a compared to Sinton and Swanson's experiment.

In this paper, we investigate a comprehensive silicon BGN model, which was recently derived by Schenk [14] from quantum mechanical principles. In contrast to previous BGN models [10,15,16], Schenk's BGN model provides the gap shrinkage for arbitrary combinations of injection and doping levels, and at temperatures between 0 and 1000 K. We demonstrate that this BGN model enables us to describe highly injected silicon much more precisely than in the past.

We use $n_i = 9.65\times10^{9}\,cm^{-3}$ in our simulations, instead of $n_i = 1.00\times10^{10}\,cm^{-3}$ reported by Sproul and Green [7], because the Schenk model influences the interpretation of n_i measurements of Sproul and Green [7], as is explained in Ref. [17]. Misiakos and Tsamakis [18] measured a value of $n_i = 9.7\times10^{9}\,cm^{-3}$ in lightly doped material, which is consistent with our value.

3. Numerical simulations in three dimensions

We implemented Schenk's BGN model in the device simulator Dessis [19], which numerically solves the fully coupled set of semiconductor differential equations in a self-consistent way. Thus, no further assumptions need to be made as to the quasi-Fermi energy levels, carrier densities, etc. Schenk's BGN model provides the band edge energies, E_c and E_v, in the whole device, including the highly doped regions. In the experiment of Sinton and Swanson, the injection density varied from 1×10^{16} to $2\times10^{17}\,cm^{-3}$, causing a gap shrinkage between 8 and 14 meV according to the model of Schenk. Using an approach reported earlier [20], we simulate the entire $3\times5\,mm^2$ cell of Sinton and Swanson in three dimensions, including 2 cm of shaded wafer material that surrounded the cell (the cell remained embedded in the wafer after fabrication). We use the experimentally known device parameters given by Sinton and Swanson [1], as listed in Table 1.

Crucial for modelling highly injected silicon is not only the choice of the three parameters n_i, BGN and C_a, but also the applied transport model. In contrast to low-injection, the mobility of free carriers depends on the relative velocity between electrons and holes [21]. For example, in the undoped regions of Sinton and Swanson's device (i.e. 99.94% of the entire volume), photo-generated electrons and holes diffuse in a parallel pattern towards the rear, and hence experience less mutual scattering events than in ohmic conduction. For such a case, the ambipolar diffusion coefficient

$$D_a = \frac{2kT}{q}\frac{\mu_n\mu_p}{\mu_n+\mu_p} \tag{2}$$

Table 1
Physical device parameters used in the simulations

Cell geometry	As published in Ref. [1]
Shaded perimeter region	2 cm from cell's edge [20]
Temperature	300 K
Illumination spectrum	AM1.5 Global [26]
Internal reflection at front surface	17% [27]
Internal reflection at rear surface	81% [27]
Contact resistance	$1 \times 10^{-6}\,\Omega\,cm^2$ [20]
Carrier statistics	Fermi-Dirac
Intrinsic electron density	$9.65 \times 10^9\,cm^{-3}$ [17]
Band gap narrowing model	Model of Schenk [14]
Mobility model	Model of Masetti et al. [23]
SRH recombination in bulk	Mid-gap traps with equal capture cross sections, lifetime $\tau = 3$ ms [1]
SRH recombination at surface	Mid-gap traps with equal capture cross sections, $S_{no} = S_{po} = 3.75$ cm/s [1]
SRH recombination at contacts	Ohmic, i.e. flat quasi-Fermi energy levels at mid-gap, equivalent to $S = \infty$ cm/s [20]
Auger coefficient	$C_a = 1.9 \times 10^{-30} - 2.8 \times 10^{-30}\,cm^{-3}$

was experimentally determined as $17.0 \pm 0.5\,cm^2/s$ [9], independent of injection density (at least up to an injection level of $1 \times 10^{18}\,cm^{-3}$ [22]). In Eq. (2), μ_n and μ_p are the mobility of electrons and holes, respectively.

As Dessis does not have a comprehensive transport model [21] for highly injected devices, we approximate the transport properties with the mobility model of Masetti et al. [23]. Although this model originally provides the drift mobility of majority carriers in low-injection (as a function of doping density), it is a reasonable approximation to the real situation in our case: the model of Masetti et al., combined with Eq. (2), yields $D_a = 16.5\,cm^2/s$ in the region of parallel carrier flow. Near the contacts, the constrained carriers have zero velocity. Thus, their scattering has the same impact on the flowing carriers as in the case of low-level injection [21], where the majority carriers are nearly at rest. Further away from the contacts, there is a region where electrons and holes do not flow in parallel, nor is one carrier constrained to zero velocity [21]. In Dessis, we are not provided with a transport model that describes this situation, which is approximated here.

4. Simulation results

With Dessis, we reproduce the steady-state V_{oc} values of Sinton and Swanson [1], and we quantify the influence of both the revised n_i and BGN on the extracted C_a.

Fig. 1a shows that our simulated short-circuit current density J_{sc} coincides with the measured values except at the highest illumination intensities where we overestimate the mobility, due to our above-mentioned approximations in the transport-model. Sinton and Swanson obtained similar behaviour with their analytical model [1]. At

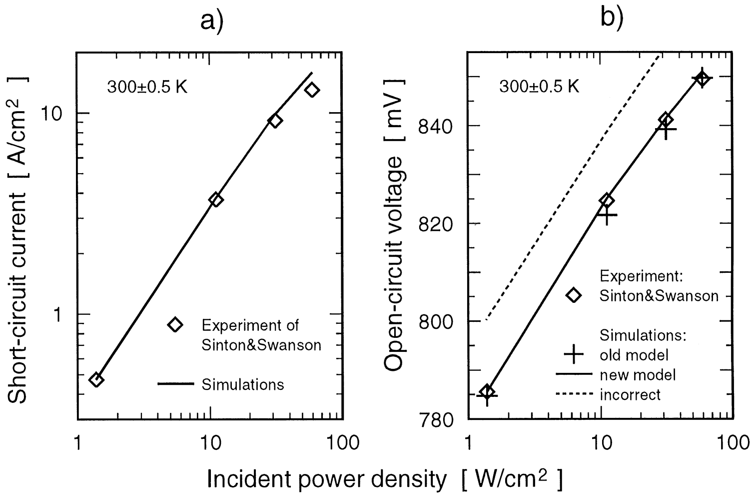

Fig. 1. Short-circuit current density (a) and open-circuit voltage (b) as a function of incident power density, measured by Sinton and Swanson [1], and simulated using the numerical model presented in this paper.

high illumination intensity, J_{sc} is very sensitive to the dimensions of the doped-regions. By optimising the device to have low uncertainties at V_{oc}, the device was made to have very high uncertainties at J_{sc}, due to the extremely high current densities from current crowding at the minimised contacts (1000 A/cm^2). These geometric uncertainties are negligible under V_{oc} conditions. The results of Fig. 1a show that our approximations in the transport model are minor, and we expect that they are even better under open-circuit conditions, where no external current-flow exists.

The V_{oc} values called ‘old model’ in Fig. 1b result from our simulations using all the parameters of Sinton and Swanson, ie. the old n_i, no BGN, and $C_a = 1.66 \times 10^{-30}\,\text{cm}^6/\text{s}$. These symbols coincide with the experimental values. Since we obtain the same V_{oc} values as Sinton and Swanson did with their analytical model, it shows that Swanson and Sinton incorporated three-dimensional effects, etc. very precisely in their analytical model. Their model is a variational approach based on emphasising the accurate determination of the total recombination current rather than carrier densities [24].

The line called ‘new model’ illustrates our simulations using the revised n_i and the BGN model of Schenk. In order to match the simulated results with the experiment, C_a has to be increased from 1.66×10^{-30} to $1.9 \times 10^{-30}\,\text{cm}^6/\text{s}$ at the highest illumination intensity, and up to 2.8×10^{-30} at the lowest illumination intensity. C_a increases with decreasing injection density because an increasing number of excitons enhances Auger recombination [12,25]. We are currently working on an injection dependent parameterisation of C_a, and we will repeat the simulations outlined in this paper with a more comprehensive description of C_a.

The dashed line in Fig. 1b called ‘incorrect’ deviates significantly from the measurements and represents simulations with the revised value of n_i but without BGN (using

$C_a = 1.66 \times 10^{-30}\,cm^6/s$). This demonstrates that choosing the revised n_i alone is insufficient. Hence free-carrier induced BGN is an important physical process in highly injected silicon, and it resolves previously experienced inconsistencies [8,9] between the revised n_i and the experiment of Sinton and Swanson.

5. Conclusions and outlook

We implemented the band gap narrowing (BGN) model of Schenk [14] in the semiconductor device simulator Dessis [19]. By reproducing the steady-state V_{oc} measurements of Sinton and Swanson [1], we demonstrated that free carrier induced BGN is an important effect in silicon concentrator cells. Using $n_i = 9.65 \times 10^9\,cm^{-3}$ [17], the BGN model of Schenk [14], and the device parameters of Sinton and Swanson [1], we had to adjust C_a in order to reproduce the measured V_{oc} values. We varied C_a from $1.9 \times 10^{-30}\,cm^6/s$ (at the highest illumination intensity) to 2.8×10^{-30} (at the lowest illumination intensity). Such an injection-dependence is expected from exciton-enhanced Auger theory [12,25], and we are currently working on an injection-dependent parameterisation of C_a in high-injection conditions.

Acknowledgements

P.P. Altermatt is on a Postdoctoral Fellowship from the Australian Research Council (ARC). He thanks H. Kim and E. Lee for generating the simulation mesh. G. Heiser's work was supported by a grant from the ARC. The Photovoltaics Special Research Centre is supported by the ARC's Special Research Centres Scheme and by Pacific Power.

References

[1] R.A. Sinton, R.M. Swanson, IEEE Trans. Electron Dev. 34 (1987) 1380.
[2] E. Yablonovitch, T. Gmitter, Appl. Phys. Lett. 49 (1986) 587.
[3] S.K. Pang, A. Rohatgi, J. Appl. Phys. 74 (1993) 5554.
[4] I.V. Grekov, L.A. Delimova, Sov. Phys. Semicond. 14 (1980) 529.
[5] P. Jonsson, H. Bleichner, M. Isberg, E. Nordlander, J. Appl. Phys. 81 (1997) 2256.
[6] M.A. Green, J. Appl. Phys. 67 (1990) 2944.
[7] A. Sproul, M.A. Green, J. App. Phys. 70 (1991) 846.
[8] E.K. Banghart, J.L. Gray, R.J. Schwartz, The effects of high level injection on the performance of high intensity, high efficiency silicon solar cells, in: Proceedings of the 20th PV Specialists Conference, Las Vegas, NV, IEEE, New York, 1988, pp. 717–722.
[9] D.E. Kane, R.A. Sinton, J.Y. Gan, R.M. Swanson, Physical parameters of highly injected silicon in the modeling of concentrator solar cells, in: Proceedings of the 21st IEEE Photovoltaics Specialist Conference, Kissemee, FL, IEEE, New York, 1990, pp. 437–441.
[10] J.R. Lowney, J. Appl. Phys. 66 (1989) 4279.
[11] E.K. Banghart, J.L. Gray, IEEE Trans. Electron Dev. 39 (1992) 1108.
[12] P.P. Altermatt, J. Schmid, G. Heiser, A.G. Aberle, J. Appl. Phys. 82 (1997) 4938.

[13] A. Neugroschel, J.S. Wang, F.A. Lindholm, IEEE Electron Dev. Lett. 6 (1985) 253.
[14] A. Schenk, J. Appl. Phys. 84 (1998) 3684.
[15] R.A. Abram, G.N. Childs, P.A. Saunderson, J. Phys. C 17 (1984) 6105.
[16] L.R. Logan, J.L. Egley, Phys. Rev. B 47 (1993) 12532.
[17] P.P. Altermatt, A. Schenk, G. Heiser, M.A. Green, The influence of a new band gap narrowing model on measurements of the intrinsic carrier density in crystalline silicon, in: T. Saitoh (Ed.), Technical Digest of the 11th International Photovoltaic Science and Engineering Conference, Sapporo, Japan, p. 719.
[18] K. Misiakos, D. Tsamakis, J. Appl. Phys. 74 (1993) 3293.
[19] ISE Integrated Systems Engineering AG, Zurich, Switzerland, Dessis Manual 4.0, 1997, http://www.ise.ch
[20] P.P. Altermatt, G. Heiser, A.G. Aberle, A. Wang, J. Zhao, S.J. Robinson, S. Bowden, M.A. Green, Prog. Photovoltaics 4 (1996) 399.
[21] D.E. Kane, R.M. Swanson, J. Appl. Phys. 72 (1992) 5294.
[22] D.E. Kane, R.M. Swanson, Electron-hole collisions in concentrator solar cells, in: Proceedings of the 20th IEEE PV Specialists Conference, Las Vegas, NV, IEEE, New York, 1988, pp. 512–517.
[23] G. Masetti, M. Severi, S. Solmi, IEEE Trans. Electron Dev. 30 (1983) 764.
[24] R.M. Swanson, Solar Cells 17 (1986) 85.
[25] A. Hangleiter, R. Häcker, Phys. Rev. Lett. 65 (1990) 215.
[26] R. Hulstrom, R. Bird, C. Riordan, Solar Cells 15 (1985) 365.
[27] J.O. Schumacher, private communication, ISE Freiburg, Germany, 1999.