The influence of a new band gap narrowing model on measurements of the intrinsic carrier density in crystalline silicon

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ABSTRACT

The commonly used value of the intrinsic carrier density of crystalline silicon, n_i=1.00(±0.015)×10^{10} cm^{-3} (at 300 K), was determined by Sproul&Green in 1991 (the value in brackets is the one-standard-deviation uncertainty). This value is the average taken from various devices with differing doping densities in the range of 1×10^{14} to 1×10^{16} cm^{-3}. Sproul&Green obtained values of n_i that increase slightly with increasing doping density. We demonstrate that their experiment was influenced by band gap narrowing, even though the doping density of their samples was low (<1×10^{16} cm^{-3}). Our re-interpretation of their measurements leads to results consistent with n_i=9.7(±0.1)×10^{9} cm^{-3}, recently determined by Misiakos&Tsamakis.

1. The n_i measurement of Sproul&Green

In 1991, Sproul&Green [1,2] determined the intrinsic carrier density of crystalline silicon, n_i, to be 1.00(±0.015)×10^{10} cm^{-3} at 300 K. Nowadays, this is the most widely accepted value of n_i in the silicon community. In their experiment, Sproul&Green designed solar cells such that their current is limited by the electron flow through the p-type base. Thus, the current-voltage (I-V) curves of these cells depend mainly on n_i, the mobility of minority electrons in the base, μ, the boron doping density in the base, N_A, and the base thickness, W. Sproul&Green obtained n_i by reproducing their measured I-V curves with an analytical model. Only n_i had to be adjusted as a free model parameter because μ, N_A, and W were known from separate measurements. The symbols in Figure 1 show the measured dark I-V curves [3], and the symbols in Figure 2 depict n_i extracted from these cells.

2. Absolute and effective intrinsic carrier density

Figure 2 suggests that the extracted n_i increases with increasing doping density. In the original work [2], it is mentioned that band gap narrowing (BGN) may be the cause for this. However, as there were no measurements available

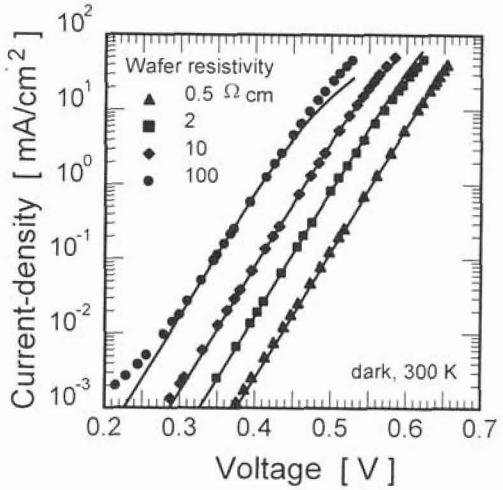

Figure 1: Dark I-V curves, measured by Sproul& Green (symbols) [2], and simulated using Dessis [6] with the BGN model of Schenk [5] (lines).

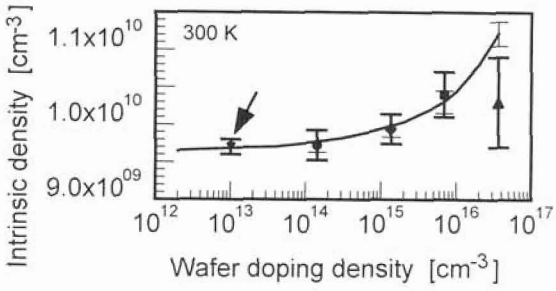

Figure 2: The (effective) intrinsic carrier density of silicon, determined by Sproul&Green with their analytical model [1] (symbols and bold error bars), the value given by Misiakos&Tsamakis [4] (arrow), and simulations with Dessis and the BGN model of Schenk [5] (line and thin error bars).

indicating BGN at N_A below 1×10^{17} cm^{-3}, the average of these n_i values was taken, ie. n_i=1.00(±0.015)×10^{10} cm^{-3}. In this paper we introduce a model that predicts a considerable amount of BGN at N_A>1×10^{13} cm^{-3}. This implies that the

values of Sproul&Green in Figure 2 do not represent n_i, but the effective intrinsic carrier density, $n_{i,eff}$, according to the formula

$$n_{i,eff}=n_i\exp[\Delta E_g/2kT] \quad (1)$$

With this interpretation, a discrepancy with the measurement of Misiakos&Tsamakis [4] is resolved, who measured n_i at carrier densities around 1×10^{13} cm^{-3} and obtained a lower value of $9.7(\pm0.1)\times10^{9}$ cm^{-3}. Their value is included in Figure 2 (arrow) and is consistent with the Sproul&Green values at low N_A. In this paper, we use the BGN model of Schenk [5], who recently developed a band gap narrowing model that is entirely derived from quantum mechanical principles and thus, in contrast to empirical BGN models, is able to calculate BGN at N_A below 1×10^{17} cm^{-3}. We implemented this model into the device simulator Dessis [6], which numerically solves the fully coupled set of semiconductor differential equations. We reproduce the dark I-V curves of Figure 1 with a simulation approach that includes the entire volume of the 2x2 cm^2 cells, including their perimeter region [7].

3. Simulation results

The lines in Figures 1 and 2 show the simulation results. The simulations deviate from the I-V measurements at high and low current-densities of Figure 1 for reasons that are well understood and explained in Ref. 1. The simulated error bars in Figure 2 (thin lines) are obtained by varying μ within the uncertainty limits of Sproul&Green's photoconductance decay measurements of μ [2] (symbols in Figure 3). The simulated error bars in Figure 2 (thin lines) are smaller than in the original work of Sproul&Green (bold lines in Figure 2) [1,2]. This is so because μ is the only parameter that is varied in our simulations, while Sproul&Green considered the uncertainties of all the other parameters as well. As our simulations imitate the measurements, they cannot reduce the uncertainties. Hence, the one-standard-deviation uncertainty of n_i used in our simulations is at least 3%, as given by Sproul&Green.

As our simulated $n_{i,eff}$ values reproduce the 'n_i values' of Sproul&Green very well (by choosing a single value of $n_i=9.65\times10^{9}$ cm^{-3}), we conclude that Sproul&Green measured $n_{i,eff}$ instead of n_i. This implies that the data of Sproul&Green and of Misiakos&Tsamakis are consistent.

4. Recommendation for n_i value

In the interpretation given here, n_i is the asymptotic value at the left part of Figure 2, ie. $n_i=9.65(\pm0.15)\times10^{9}$ cm^{-3}. In most cases, it does not make a substantial difference whether $n_i=9.65(\pm0.15)\times10^{9}$ cm^{-3} or $1.00(\pm0.015)\times10^{10}$ cm^{-3} is used. These values differ only by 4%. If calculations are made with a BGN model that yields no gap shrinkage below a dopant density of 1×10^{17} cm^{-3}, and the behaviour of the device is ruled by a region with a resistivity of 1-10 Ωcm, one may use $n_i=1.00(\pm0.015)\times10^{10}$ cm^{-3}, as this value is the actual $n_{i,eff}$ of this region. This is the case for many types of solar cells, and explains why $n_i=1.00\times10^{10}$ cm^{-3} has been so successfully applied even in highly accurate simulations [7]. If the BGN model of Schenk is applied, we recommend using $n_i=9.65(\pm0.15)\times10^{9}$ cm^{-3}. In cases where the behaviour of the device is ruled by highly doped regions, care must be taken that the applied BGN model was derived with a similar n_i value as is used in the simulations. Otherwise, the BGN model has to be adjusted to the new n_i value. For more details, please refer to the paper of Schumacher *et al.* of this conference.

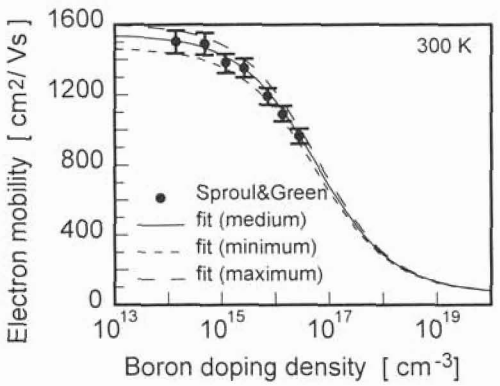

Figure 3: The minority electron mobility, measured by Sproul&Green [2] (symbols), and three parameterisations used in our Dessis model (lines).

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