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Towards a unified low-field model for carrier mobilities in crystalline silicon

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ABSTRACT

The electrical properties of crystalline silicon crucially depend on the mobility of minority and majority charge carriers. As parameters like the conductivity and the diffusion length are directly connected to carrier mobility, its exact prediction is essential for device simulation and material characterization. While generally accepted mobility models exist for uncompensated silicon, strong deviations have been observed in compensated silicon depending on the compensation level. Different approaches have been suggested for modeling majority carrier mobility correcting for compensation. In this work, the controversially discussed physical reasons for mobility reductions in compensated silicon are critically reviewed and we present a unified description of mobility in silicon. Based on the approach suggested by Schindler et al. [Solar Energy Materials and Solar Cells 106 (2012) 31–36], which describes the modeling of majority carrier mobilities in p-type compensated silicon at room temperature, the model is extended to both majority and minority carrier mobilities in p- and n-type compensated silicon at room temperature and a description for the temperature dependence is suggested. Fit parameters are obtained based on a wide range of published and new carrier mobility data presented here. Additionally, a new parameterization for scattering of holes by phonons is presented and included in the model.

1. Introduction

Although accounting for the simultaneous presence of acceptors and donors as scattering centers, Klaassen's mobility model [1] fails to correctly describe carrier mobilities in compensated silicon [2–12]. As Klaassen's model is based on the empirical mobility expression of Caughey and Thomas [13] developed for uncompensated silicon, and parameters are obtained from fitting experimental data in uncompensated silicon, not quite unexpected deviations are found for compensated silicon. It has been shown in several publications, e.g. [10,11], that the deviation from Klaassen's model depends on the compensation level. In a previous work [10], reduced mobilities are explained by reduced screening which is not sufficiently taken into account in Klaassen's model. This assumption is challenged by temperature dependent measurements in other publications [8,11], suggesting that reduced screening alone cannot explain mobility reductions along the whole temperature range.

In this work we show that temperature dependent measurements do not necessarily contradict the hypothesis of reduced screening as a reason for mobility reductions. The approach suggested in [10] is used as a starting point for a unified description of mobilities in compensated silicon. We first show that a single set of parameters can be used for the description of both majority hole and electron carrier mobility in compensated silicon at room temperature. Using the same parameter set and introducing an additional dependence on the total dopant concentration also allows for modeling minority electron and hole mobility. In a third step, the model is extended to correctly describe mobility data in compensated silicon along the temperature range from 80 to 350 K including a new phenomenological parameterization for hole scattering at phonons. Thus, a unified mobility model is obtained, which merges with Klaassen's mobility model including

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a new parameterization for hole scattering at phonons in the case of uncompensated silicon.

2. Physical motivation and approach

In order to motivate the approach presented in this work, some remarks are required regarding the origin of mobility reductions in compensated silicon. Mobility reductions in compensated silicon have been frequently observed in the past years [2–12]. The reasons were controversially discussed and different approaches to account for these mobility reductions were suggested. In [6], a mobility correction term $\mu_{cor} \propto C_l^{-3/4}$, C_l denoting the compensation level, attributed to a specific compensation effect which is not taken into account in the existing mobility models is suggested. Adding such a correction term according to Matthiesen's rule $(1/\mu = 1/\mu_{Klaassen} + 1/\mu_{cor})$ can only be justified with an additional scattering channel in compensated silicon, which has not been proven to exist so far. In [9] it is argued that the discrepancy of experimental and modeled mobility values in compensated silicon highlights the non-physical character of Klaassen's model rather than a mobility reduction due to compensation as Klaassen's model is based on a substantial amount of fitting to data in uncompensated silicon. A correct mobility description would therefore require a complete re-assessment of Klaassen's fitting parameters. Alternatively, a very simple empirical correction for compensation is suggested in that work: by multiplying Klaassen's mobility with a prefactor depending on the compensation level and the type of carrier, a good description of mobility in compensated silicon can be achieved. While the simplicity is the strength of this correction, its weakness is its purely empirical nature.

An approach previously put forward by some of the authors attempted to stay as close as possible to the largely successful Klaassen's model [10]. As an explanation for reduced mobilities in compensated silicon a reduction of screening that is not accounted for sufficiently in Klaassen's model was introduced. By adding a compensation-dependent term accounting for reduced screening in the Caughey–Thomas mobility expression, which is the empirical starting point in Klaassen's model, we tried to keep the physical character of the model. However, temperature dependent measurements appeared to contradict this hypothesis, as reducing the temperature increases the compensation level without a further strong mobility reduction [8]. A closer look at the implementation of the *T*-dependence of impurity scattering in Klaassen's model [14] allows for solving this apparent contradiction

$$\mu_{i,I} = \frac{\mu_{max}^2}{\mu_{max} - \mu_{min}} \left(\frac{N_{ref,1}}{N_I}\right)^{\alpha_1} \left(\frac{T}{300\ \text{K}}\right)^{3\alpha_1 - 1.5} + \frac{\mu_{min} \cdot \mu_{max}}{\mu_{max} - \mu_{min}} \left(\frac{c}{N_I}\right) \left(\frac{300\ \text{K}}{T}\right)^{0.5} \quad (1)$$

The second term in this equation accounts for reduced screening with decreasing carrier concentration c at a constant concentration of ionized scattering centers N_I. As argued in [10], at room temperature the first term is predominant for dopant concentrations $N \le N_{ref} = 2.23 \times 10^{17}\ \text{cm}^{-3}$, i.e. reduced screening is not taken into account adequately in Klaassen's model in this dopant range. With decreasing temperature, however, the second term becomes more important (e.g. at 100 K, the first term is reduced to 50% of its room-*T* value, while the second term is roughly doubled). This means, the lower the temperature, the more Klaassen's model already accounts for reduced screening in compensated silicon without any correction. Therefore, comparing mobilities with Klaassen's model for the case of an increased compensation level by doping at room temperature and for the case of increased compensation level by a temperature reduction is actually expected to lead to a completely different behavior. Consequently, temperature dependent mobility measurements in compensated silicon are not necessarily in contradiction with the assumption of reduced screening as a reason for reduced mobilities at room temperature. Therefore, in this work we follow the approach presented in [10] to install a mobility model predicting mobilities in uncompensated and compensated silicon. Our reasoning to put this approach forward is that the introduction of the compensation-dependent correction term in the empirical Caughey–Thomas expression can at least be physically motivated.

In the first part we will extend the model presented for majority hole mobilities in compensated p-type silicon [10] to majority and minority hole and electron mobilities in compensated p- and n-type silicon and obtain the fit parameters from a larger data base including new mobility data in compensated silicon. In the second part we will discuss the temperature dependence of majority carrier mobilities in compensated silicon from 80 to 350 K including a new parameterization of the phonon-scattering. Details on the model implementation are summarized in Appendix C.

3. Results

3.1. Modeling mobility at room temperature

3.1.1. Majority hole and electron mobility

In this section we present new majority hole and electron mobility data in compensated p- and n-type silicon, obtained from Hall measurements on different materials at two different institutes. Details on the measurement techniques at Fraunhofer ISE can be found in [15], details on the measurement techniques used by Apollon Solar in [8]. Dopant concentrations and measured mobilities which have not been published so far are listed in Appendix A. Fig. 1a presents the data (colored symbols) plotted as relative deviation from Klaassen's model as a function of the compensation level $C_l = (N_A + N_D)/c$, where $N_A + N_D$ is the sum of ionized acceptors and donors and c the free carrier concentration $n_0 + p_0$. Note that all data presented in this work was obtained from experiments without injection of carriers for majority carrier measurements and under low injection of carriers for minority carrier measurements. Additionally we include data from reference [11], which were not considered yet by the model fit done in [10].

These new data follow the same trend as the earlier published data (plotted as gray crosses) collected in [10], and, remarkably, relative deviations from Klaassen's model are the same for majority hole and majority electron mobility, measured on compensated p-type and n-type silicon respectively. Following the approach presented in [10], we use a modified Caughey–Thomas mobility expression

$$\mu = \frac{\mu_{max} - \mu_{min}}{1 + (N/N_{ref})^{\alpha} + ((C_l - 1)/C_{l,ref})^{\beta_1}} + \mu_{min} \quad (2)$$

as a starting point for Klaassen's model. Details on the implementation can be found in [10] and in Appendix C. The fit parameters $C_{l,ref}$ and β are adjusted for the majority hole and electron mobilities by additionally taking these new mobility data into account

$$C_{l,\ ref} = 24.82 \pm 2; \quad \beta_1 = 1.092 \pm 0.03 \quad (3)$$

Note that mobility data from [4], which had been considered in the fitting in [10], is neglected in this work. In [4], compensation was achieved by activation of thermal donors, thereby introducing doubly ionized scattering centers. When plotted as a function of the compensation level, these mobility data show a significantly larger spread than mobility data from compensated material solely containing singly charged scattering centers. The larger spread can be due to several reasons. On the one hand, the scattering power