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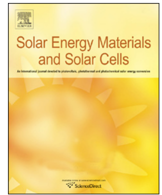

Interstitial oxygen imaging from thermal donor growth—A fast photoluminescence based method

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ABSTRACT

We present a fast method to create interstitial oxygen concentration maps from resistivity calibrated photoluminescence images prior to and after a heat treatment at 450 °C. The method utilizes the influence of thermal donors on the effective doping concentration of a sample. Although the determination of thermal donor concentrations from conductivity measurements is customary in literature, we found that implementation of a mobility model is necessary to determine accurate concentrations of thermal donors. Therefore an iterative correction algorithm is presented, which allows precise determination of thermal donor concentrations from resistivity measurements. The determination of interstitial oxygen concentrations from thermal donor concentrations is based on an updated parameterization based on a model of Wada et al. (Phys. Rev. B: Condens. Matter 30 (1984) 5884–5895) that is also presented in this paper. The method is demonstrated on a 1.3 Ω cm p-type Czochralski grown silicon sample with an interstitial oxygen concentration in the range of 7.5×10^{17} cm^{-3} and yields good agreement with FTIR measurements.

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1. Introduction

Oxygen is usually introduced into the silicon crystal during crystal growth and can be present in concentrations up to the range of 10^{18} cm^{-3} in silicon grown with the Czochralski method. High interstitial oxygen concentrations ($[O_i]$) can give rise to the growth of oxygen complexes called thermal donors (TD) [1] or new donors [2,3] and recombination active oxide precipitates [4] during high temperature treatments. In the presence of boron, e.g. in standard p-type silicon, interstitial oxygen forms complexes that are responsible for light induced degradation [5,6]. Thus, the determination of the oxygen content of silicon wafers is crucial for quality control and process design in photovoltaic production as well as for many investigations on crystal defects.

The most widespread and well established way to determine $[O_i]$ is to evaluate characteristic infrared absorption measured with Fourier transform infrared spectroscopy (FTIR). Veirman et al. [7] have presented an alternative measurement technique that is based on monitoring the change of the conductivity of wafers due to TD growth after a 450 °C tempering step. This method is also capable of performing lateral scans of $[O_i]$ with scanning 4-point-probe measurements. Both methods are limited in resolution and are time consuming on relevant sample sizes.

In this paper, we utilize resistivity calibrated photoluminescence (PL) images [8] to perform high resolution $[O_i]$ images in a strongly reduced time. Also, a necessary correction for the influence of TDs on carrier mobilities in silicon is introduced utilizing a recent model by Schindler et al. [9].

2. Method

2.1. Working principle

The method is applied to as-cut wafers after a temperature step at or above 850 °C to dissolve all TDs already present in the material from crystal growth. In this temperature range, the formation of new donors is not expected [3] and therefore the electrical properties of the wafer should be determined by the sample doping. Afterwards, the sample undergoes hot DI water etching to achieve a high surface recombination velocity [10]. For very high surface recombination velocities, the excess carrier density Δn is determined by the time necessary to reach the surface (transit time) instead of bulk charge carrier lifetime. In this case (surface limitation of Δn), PL intensity is proportional to the effective doping concentration [8]. Without compensation

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effects, e.g. from TDs in p-type silicon, this corresponds to the dopant concentration and the PL image can be calibrated with local conductivity data from e.g. four-point-probe measurements to a doping image [8]. In order to create TDs, the sample is subjected to an annealing step at 450 °C for several hours, which gives rise to TD formation [1].

After the annealing step the aforementioned surface treatment is repeated and a second PL image is taken. This image and resistivity measurement to calibrate it will be influenced by the created TDs due to their electronic structure. A detailed insight into these influences and an algorithm to account for them will be given in Section 2.2. Taking these influences into account, the second PL image can be calibrated to an effective doping image. As the difference between the doping image (before annealing) and the effective doping image (after annealing) results solely from the presence of TDs, an image of their concentration N_{TD} can be calculated by considering their charge state, which can be assessed with the algorithm as well.

The formation kinetics of TDs is highly dependent on the initial $[O_i]$. We have combined features of parameterizations by Wada et al. [11] and Wijaranakula [12] into a new model that is presented in Section 2.3. Utilizing this new parameterization, we calculate high resolution $[O_i]$ images for a given annealing treatment defined by temperature T and duration t from the previously calculated N_{TD} images. Fig. 1 briefly illustrates the process steps of the presented method.

2.2. Precise determination of thermal donor concentration

As the method is based on the evolution of TD concentration, its precise determination is crucial. TDs act as donors and thus it appears convenient to determine N_{TD} from conductivity measured in a TD-free state (i.e. after a high temperature step) of the sample, $\sigma_{withoutTD}$, and after intentional formation, σ_{meas}. Because the electronic properties of TDs differ from common dopants, such as boron or phosphorus, special care has to be taken, in order to determine their actual concentration.

TDs introduce two energy states in the bandgap of silicon close to the conduction band [13]. The exact position of these states is determined by the number of oxygen atoms included in the TD, but the most common sizes of TDs create levels in a narrow energy range [14]. Therefore their charge state (*TDcharge*) is dependent on the position of the Fermi energy E_F following Fermi–Dirac-Statistics. In p-type silicon TDs will always act as double donors and thus compensate the sample doping. In n-type samples, the charge state of TDs will depend on the position of E_F relative to the energy states of TDs and therefore on the doping concentration (N_{dop}) and also on N_{TD}. Furthermore, multiply charged defects and donor compensation have a strong impact on charge carrier mobilities of minority and majority charge carriers μ_{min} and μ_{maj}. As Schindler et al. [9] pointed out, the influence of compensation effects can reduce the mobilities by up to 50% compared to widely used models. To account for these influences, we have developed an algorithm, that utilizes Klaassen's model for charge carrier mobilities [15,16] with additions for compensation effects by Schindler [9] and an iterative method to determine N_{TD} and *TDcharge*.

The necessary input parameters for the algorithm are the actual doping concentration N_{dop} (N_A in p-type, N_D in n-type) and the measured conductivity σ_{meas} of the sample including TDs. In the case of compensated silicon, both dopant concentrations have to be known. The first step is to determine an apparent doping concentration N^*_{dop} from σ_{meas} by neglecting the additional influences of TDs on carrier mobilities, similar to a common *resistivity-to-doping* calibration. The difference between N_{dop} and N^*_{dop} divided by two serves as a first estimate of N_{TD} and as starting value for the iterative algorithm. It should be mentioned that most research on TD evolution in the past neglected the difference between this estimate and the actual N_{TD}.

The algorithm calculates charge carrier mobilities $\mu_{min,i}$ and $\mu_{maj,i}$ from $N_{TD,i}$ and $TDcharge_i$ according to Schindler's model. Then it determines the charge carrier concentrations $p_{0,i}$ and $n_{0,i}$, to reproduce σ_{meas}. The carrier concentrations lead to $N_{TD,i+1}$ and $TDcharge_{i+1}$ using common charge carrier statistics. Fig. 2 shows a schematic illustration of the computational steps. We found in simulations that few iterations of this process lead to precise

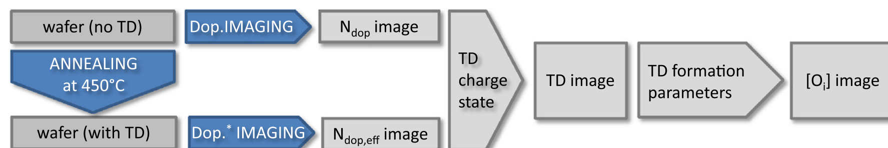

Fig. 1. Schematic illustration of the measurement and evaluation.

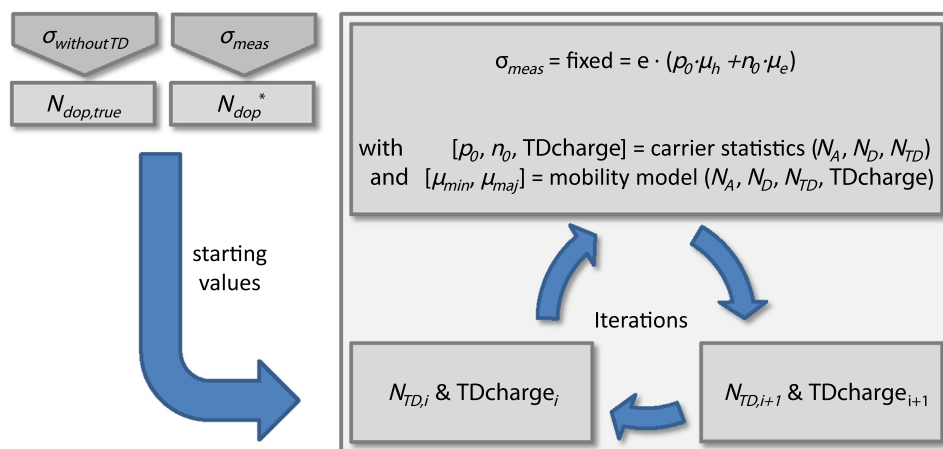

Fig. 2. Schematic illustration of the mobility correction tool. Starting from conductivity measurements before and after annealing ($\sigma_{withoutTD}$ and σ_{meas}) a set of parameters is calculated for an iterative algorithm resulting in the true TD concentration and their charge state.

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