Temperature Dependent Mobility Model for Predictive TCAD Simulations of 4H-SiC

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Abstract. We present a calibrated bulk mobility model for 4H-SiC. Hall measurements are performed on 4H-SiC samples to determine the bulk mobility/resistivity in the temperature range of 200-500K. We observe that temperature dependence of bulk resistivity cannot be predicted by popular mobility models available within TCAD tools. A careful investigation reveals that these popular mobility models need to be revised and replaced by a comprehensive model that can describe the impurity scattering effects dominant at low temperatures. We present a well calibrated bulk mobility model for 4H-SiC exhibiting excellent agreement with measured data, making it suitable for device simulation purposes using TCAD tools.

Introduction

Silicon Carbide (SiC) based MOSFETs are quickly becoming the workhorse switch in power electronics applications due to their low on-state resistance, faster switching and ability to operate at higher temperature than Si counterparts. There is a growing demand for SiC technology from a wide range of applications that includes electric vehicles, solar inverters, power supplies, industrial motor drives and energy storage etc. To meet these demands and enhance the efficiency of devices, research & development efforts have been put into the design and development of next generation SiC devices. The success of these efforts critically depends on the ability to describe the SiC material system with reliable and precise electrothermal models. Particularly, Technology Computer Aided Design (TCAD) simulations for modeling and design of next generation devices requires an accurate description of carrier concentration and corresponding mobility, as a function of temperature and applied electric field. Popular choices of bulk-mobility models used for the 4H-SiC material system are the Caughey-Thomas (CT) and Arora mobility models [1-4]. These models are successful in describing the mobilities for a wide range of carrier concentrations (1x10¹⁴-1x10²¹cm⁻³) and temperatures above room temperature (> 300K). However, they are found to be inadequate to describe the low-temperature (< 300 K) behavior of carrier mobility, as observed in Hall measurements. In this work, we focus on identifying the correct mobility model to enable the existing framework for predictive simulations.

Experimental and Simulation Method

Hall measurements are performed on high-quality low resistivity nitrogen doped 4H-SiC substrates sourced from standard 150 mm Wolfspeed SiC wafers. The measurements are done on Siface (0001) oriented samples cut 4° off-axis. Here, we considered two samples with distinct doping concentrations of 5.8×10^{18} and 4.5×10^{18} cm⁻³, respectively, as determined using SIMS profiles (see Figure 1). Hereafter, these will be referred as 'Sample 1' and 'Sample 2'. The temperature dependences of the active carrier concentrations for these two samples, measured using the Hall experiments, are shown in Figure 2. Simulations are performed using the SILVACO TCAD [7].

Results and Discussion

Carrier concentration fit using the Incomplete ionization model:

In an operational device, the active carrier concentration is a function of temperature and to model such behavior an incomplete ionization model is used which describes the rate of activation. Typically, active dopant concentration increases with increasing temperature until complete ionization is achieved. For nitrogen doping, we used a two-level incomplete ionization model and corresponding TCAD fit using this model is also shown in Figure 2. Within the 4H-SiC lattice, we have hexagonal and cubic sites and depending on whether the dopant nitrogen atom is sitting at the hexagonal site or cubic site, the ionization energy changes. The two-level model accounts for this difference. Furthermore, as the dopant concentration is increased, the distinct energy levels overlap and form a impurity band that effectively reduces the band gap of 4H-SiC crystal and is known as band gap narrowing effect. We observe that at high doping concentrations of 5.8x10¹⁸ and 4.5x10¹⁸cm⁻³, the bandgap narrowing effect is strong and it lowers the incomplete ionization energies.

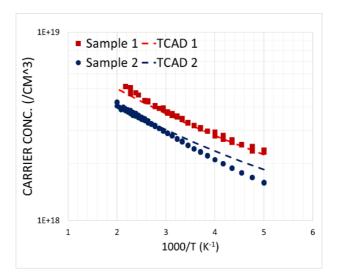


Figure 1: SIMS profile for two Samples (1 and 2) of 4H-SiC substrate with different resistivities.

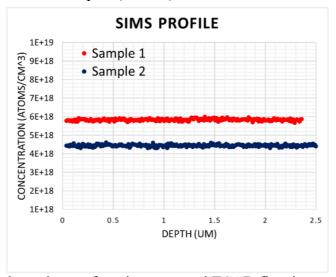


Figure 2: Temperatue dependence of carrier conc. and TCAD fit using an incomplete ionization model.

Bulk mobility using conventional models:

The Hall resistivity as a function of temperature is shown in Figure 3, using the markers for the two samples measured. We observe that the Hall resistivity, starting around 200K, initially decreases with increasing temperature and reaches a minimum value around \sim 400K for Sample 1 and \sim 370 K

for Sample 2. Thereafter, the resistivity of both the samples steadily increases with increasing temperatures. Here, we can broadly define two regions – low temperature region between 200-350 K where the resistivity decreases and high temperature region between 350 – 500 K and beyond, where it increases with increasing temperature. In order to model this behavior in TCAD, we have used popular mobility models (the Caughey-Thomas (CT) and Arora mobility model). Mobility from the CT model is described by:

$$u_{T} = u_{min} * \left(\frac{T}{300}\right)^{\alpha} + \frac{u_{max} * \left(\frac{T}{300}\right)^{\beta} - u_{min} * \left(\frac{T}{300}\right)^{\alpha}}{1 + \left[\left(\frac{T}{300}\right)^{\gamma} * \left(\frac{N}{Ncrit}\right)^{\delta}\right]}$$

Here ' u_T ' is the mobility at temperature 'T', u_{min} and u_{max} are minimum and maximum values of mobility, 'N' is the doping concentration 'N_{crit}' and the coefficients ' $\alpha, \beta, \gamma, \delta$ ' are empirical fitting parameters.

The Arora model has a similar form and is described by:

$$u_{T} = u_{min} * \left(\frac{T}{300}\right)^{\alpha} + \frac{u_{max} * \left(\frac{T}{300}\right)^{\beta}}{1 + \left(\frac{300}{T}\right)^{\gamma} * \frac{N}{N_{crit}}}$$

The predictions for bulk resistivity and mobility, using the CT model, are shown in Figure 3 and 4, respectively. Similar results are also obtained with the Arora model and are omitted from these graphs for clarity. The TCAD simulations based on the CT model predict a monotonic increase in bulk resistivity with increasing temperature (similar trend also observed using the other model). Thus, this mobility model is unable to describe the low temperature behavior of the substrate resistivity as seen in the Hall measurements. A careful analysis of the model reveals that - this model does not include the impurity scattering terms that are dominant at low temperatures. Carrier mobility is a complex phenomenon and a variety of scattering mechanism should be included as per Matthiessen's rule. The temperature effects described by the CT or Arora models are only able to describe the impact of lattice scattering that dominates at higher temperature. Therefore, we have investigated other more comprehensive bulk mobility models that have been developed for Si technology.

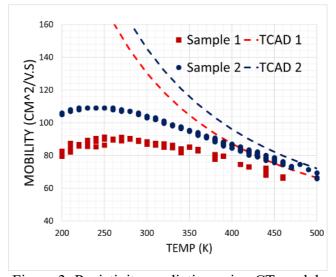


Figure 3: Resistivity prediction using CT model.

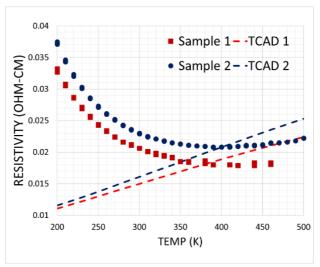


Figure 4: Mobility fit using the CT model.

Bulk mobility using Klaassen model:

Our review of existing bulk mobility models which include the impurity scattering term suggests that the unified Klaassen mobility model [5,6] is the most comprehensive approach. Thus, we chose to work with this model to describe the bulk mobility of 4H-SiC. Within this model, the total low-field mobility is the combination of two main components: first is the lattice scattering (L) term and the second term represents donor (D), and/or acceptor (A) carrier-carrier scattering as well as screening effects (P), combined using Matthiessen's rule:

$$\frac{1}{u} = \frac{1}{u_L} + \frac{1}{u_{DAP}}$$

This mobility model contains over 20 parameters and thus allows for a greater flexibility to address the individual scattering terms. We have evaluated and calibrated these scattering terms (originally proposed for Si) for 4H-SiC. The predicted resistivity and mobility curves using the calibrated Klaassen model, are shown in Figure 5 and 6, respectively, along with measured data. The results show good agreement with the Hall measurements, also predicting the maximum value (cusp) for the mobility around ~250 K and ~270 K in the curves corresponding to two samples having different doping concentrations.

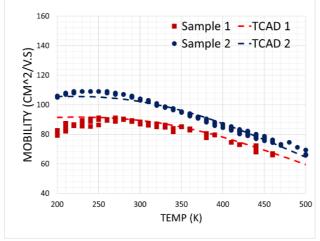


Figure 5: Resistivity prediction using Klaassen model.

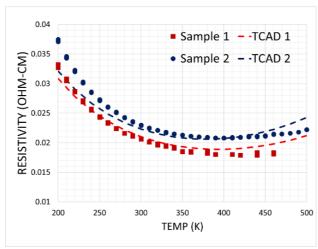


Figure 6: Mobility fit using the Klaassen model.

Summary and Conclusions

In this paper, we have presented Hall measurements for nitrogen doped 4H-SiC substrate for bulk mobility and resistivity. A two-level incomplete ionization model, that accounts for band gap narrowing effect, successfully described the temperature dependence of the active carrier concentrations. We observe that the popular mobility models, such as the CT or Arora models, only include lattice scattering terms and therefore are only useful at higher temperatures (> 300 K). For lower temperature (< 300 K) they are not able to represent the Hall measurements. A comprehensive model, that includes the impurity scattering effects, is needed to describe the temperature and concentration dependence of substrate resistivity as measured in Hall experiments. We presented a calibrated Klaassen bulk mobility model for the 4H-SiC system and the results are in excellent agreement with Hall measurements, both qualitatively and quantitatively. We also emphasize that the model suggested is of importance when considering the thermal coefficient of resistivity across a wide range of temperature from -55°C up to 225°C and beyond. In conclusion, our TCAD framework of revised understanding of the incomplete ionization and the extended mobility model can accurately predict the temperature dependence of the resistivity and mobility of highly doped 4H-SiC substrate.

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