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Numerical modelling of polycrystalline diamond device for advanced sensor design

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Abstract

Technology Computer Aided Design (TCAD) simulation tools are routinely adopted within the design flow of semiconductor devices to simulate their electrical characteristics. However, the device level simulation of diamond is not straightforward within the state-of-the-art TCAD tools. Physical models have to be specifically formulated and tuned for single-crystal CVD (scCVD) and polycrystalline (pcCVD) diamond in order to account for, among others, incomplete ionization, intrinsic carrier free material, dependences of carrier transport on doping and temperature, impact ionization, traps and recombination centers effects.
In this work, we propose the development and the application of a numerical model to simulate the electrical characteristics of polycrystalline diamond conceived for sensors fabrication. The model is based on the introduction of an articulated, yet physically based, picture of deep-level defects acting as recombination centers and/or trap states. This approach fosters the exploration and optimization of innovative semiconductor devices conjugating the capabilities of CMOS electronics devices and the properties of diamond substrates, e.g. for biological sensor applications or single particle detectors for High Energy Physics experiments.

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Keywords: TCAD; Numerical Modelling; Diamond

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1. Introduction

Synthetic diamond exhibits electrical properties such as low dielectric constant and low losses, a high electrical carrier mobility and a wide electronic bandgap, fostering its application in electronics device and circuit design and fabrication. Within this framework, Technology Computer Aided Design (TCAD) simulation tools are routinely adopted, to simulate device and circuit electrical characteristics, as a response to external stimuli. However, the device level simulation of diamond is not straightforward within the state-of-the-art TCAD tools such as Synopsys© TCAD (Sentaurus). Physical models have to be specifically formulated and tuned for single-crystal CVD (scCVD) and polycrystalline CVD (pcCVD) diamond in order to account for, among others, incomplete ionization, intrinsic carrier free material, dependences of carrier transport on doping and temperature, impact ionization, traps and recombination centers effects.

In this work, we propose the development and the application of a numerical model to simulate the electrical characteristics of pcCVD diamond conceived for innovative sensors fabrication. The model is based on the introduction of an articulated, yet physically based, picture of deep-level defects acting as recombination centers and/or trap states. This approach fosters the exploration and optimization of innovative semiconductor devices conjugating the properties of diamond substrates and the functionalities of CMOS electronics devices.

2. TCAD diamond parameter setup

Diamond is a “novel” material for device-level numerical simulation tool; it is therefore necessary to add a new custom-defined semiconductor to the material library of the TCAD tool at hand, namely the Synopsys© Advanced TCAD Sentaurus. The main parameters of scCVD have been collected from literature and incorporated within the material definition. Among others, the wide band-gap, the exceptionally high carrier mobility, the high critical electric field, which make the diamond suitable for high-voltage and high-temperature applications [1, 2, 3].

However, aiming at “smart” electronics circuit and system design, the activation of dopants is an important issue that should be addressed for the application of diamond devices. It originates from the wide diamond bandgap, responsible for the large ionization energies of dopants in the material. The incomplete ionization still limits the number of carriers which can be introduced into the valance band with increasing dopant concentrations [4].
In this work an incomplete ionization model has been considered [5] by means of the following equations, which represent the concentration of ionized impurity atoms:

$$N_D = \frac{N_{D,0}}{1 + g_D \exp\left(\frac{E_{F,n} - E_D}{kT}\right)}, \quad for\ N_{D,0} < N_{D,crit} \qquad N_A = \frac{N_{A,0}}{1 + g_A \exp\left(\frac{E_A - E_{F,p}}{kT}\right)}, \quad for\ N_{A,0} < N_{A,crit}$$

where $N_{D,0}$ and $N_{A,0}$ are the donor and acceptor concentration, g_D and g_A are the degeneracy factors for the impurity levels and E_D and E_A are the donor and acceptor ionization (activation) energies. The $N_{D,crit}$ and $N_{A,crit}$ values were taken from [1]. The density-of-states for the conduction and valence bands (N_C and N_V) that influence the intrinsic carrier concentration have been set to $N_C = 5.0\times10^{18}$ cm^{-3} and $N_V = 1.8\times10^{19}$ cm^{-3} at 300K [3]. Boundary conditions and contact properties have to be set up as well. To this purpose, it should be mentioned that the electron affinity depends highly on the nature of the surface termination. In the experimental devices diamond surfaces are typically treated with an oxygen plasma (X_0 = 1.7 eV) or hydrogen plasma (X_0 = -1.3 eV) prior to contact realization [6].

With the aim of validating the parameter choice, in Fig. 1 is represented the comparison between the incomplete ionization model and the simulation results that have been obtained by means of steady-state simulations. Fig 2 shows a comparison between the simulated hole mobility as a function of the boron concentration and experimental results.

Once assessed the main parameters of the “new” material representing the scCVD diamond within the TCAD tools, a number of issues are still to be addressed for an efficient steady-state and transient (time-variant) analysis. In particular, the very low intrinsic concentration of the diamond, in the order of $n_i = 10^{-27}$ cm^{-3} at 300K, is unsuitable for typical TCAD solvers, because leads to numerical analysis issues. Possible strategies to cope with this issue are the following: