

MODEL OF CARRIER MULTIPLICATION DUE TO IMPURITY IMPACT IONIZATION IN BORON-DOPED DIAMOND

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Abstract

Boron-doped diamond exhibits a characteristic S-shaped I-V curve at room temperature [1] with two electrical conductivity states, i.e., low and high conductivity, at high electric fields (50 - 250 kVcm⁻¹) due to the carrier freeze-out and impurity impact ionization avalanche effect. To our knowledge, the carrier multiplication during the change of the conductivity state has not been studied. In this article, we investigate theoretically the effect of acceptor concentration and compensation level on the carrier multiplication coefficient at room temperature to determine the optimal dopants concentration of maximum carrier multiplication. The room temperature hole concentration of boron-doped diamond has been calculated for various acceptor concentration and compensation ratio by solving numerically the charge neutrality equation within the Boltzmann approximation of the Fermi-Dirac statistic. These values were used to determine theoretical carrier concentration multiplication coefficients as a function of the acceptor concentration and compensation ratio. The calculated multiplication coefficient is maximum for an acceptor concentration of ca. $2 \cdot 10^{18}$ cm⁻³ and it increases with the compensation above 0.2 %. These theoretical values are consistent with the ratio of the carrier concentration at room temperature and the acceptor concentration available in the literature as well as the current multiplication observed in boron-doped diamond due to impurity impact ionization avalanche [1].

Keywords: Boron-doped diamond, semiconductor, carrier multiplication coefficient, impurity impact ionization

1. INTRODUCTION

The high ionization energy of electrically active dopants is one of the specificities of diamond as a semiconductor. As a result, the carrier freeze-out regime, i.e, the region of incomplete ionization of the dopants, extends towards temperatures well above “normal” operation temperature. The complete ionization of the dopant can be achieved within this temperature range by impurity impact ionization avalanche. This effect, first studied in germanium at cryogenic temperature, has been recently observed in boron-doped diamond in a wide range of temperature and in a wide range of acceptor concentration [1,2]. In this article, we investigate theoretically the effect of acceptor concentration and compensation level on the room temperature's carrier multiplication coefficient to determine the optimal theoretical dopants concentration to obtain maximum carrier multiplication attainable by impurity impact ionization avalanche effect.

2. MODEL

In this work, the carrier multiplication coefficient is defined as the ratio between the carrier concentration at complete ionization of acceptors, i.e., $N_a - N_d$ with N_a the acceptor concentration and N_d the compensating donor

concentration, and the carrier concentration at a given operating temperature, room temperature in this work. The carrier concentration is determined by solving numerically the charge neutrality equation within the Boltzmann approximation of the Fermi-Dirac statistic, i.e., assuming a non-degenerated semiconductor. The key parameters in the determination of the hole concentration (p) in boron-doped diamond are the effective density of states of the conduction (N_c^*) and valence (N_v^*) bands, the acceptor degeneracy factor (g_a), and the acceptor activation energy (E_a) [3]. In this work, the density of states and the degeneracy factor values are assumed to be independent of the acceptor concentration. The activation energy of dopants in semiconductors varies with their concentration [4]. In this work, we use the model proposed by Pearson and Bardeen [4] to model the activation energy dependence using equation (1):

$$E_a = E_I - \alpha \cdot N_a^{1/3} \quad (1)$$

Where:

E_I - the ionization energy of an isolated boron acceptor (eV).

E_a - the acceptor activation energy (eV)

N_a - the acceptor concentration (cm^{-3})

The parameter α was determined assuming the Mott transition occurring at an acceptor concentration of $2 \cdot 10^{20} \text{ cm}^{-3}$. All parameters used in this work are reported in **Table 1**.

Table 1 List of parameters used to numerically determine carrier concentration

N_c^* (300 K)	N_v^* (300 K)	g_a	E_I	α
10^{20} cm^{-3}	10^{19} cm^{-3}	6	0.370 eV	$6.3 \cdot 10^{-8} \text{ eV.cm}$

3. RESULTS

Figure 1 shows the Arrhenius plot of the calculated hole concentration in a boron-doped diamond with an acceptor concentration of $3 \cdot 10^{18} \text{ cm}^{-3}$ for various concentration of compensation impurities. This figure clearly shows that diamond is in the carrier freeze-out regime for temperature as high as 1000 K and above. The carrier concentration at room temperature is nearly independent of the concentration of compensation impurities below $3 \cdot 10^{15} \text{ cm}^{-3}$, but it significantly decreases above this threshold value. Hence, the compensation can significantly increase the carrier multiplication coefficient without noticeably reducing the carrier concentration in complete acceptor ionization conditions. **Figure 2** shows the calculated room temperature carrier concentration multiplication coefficient for various boron concentration and percentage of compensation impurities. This calculation has been limited to acceptor concentration below 10^{20} cm^{-3} to remain within the Boltzmann approximation of the Fermi-Dirac statistic. This figure shows there is a maximum of the carrier multiplication coefficient for an acceptor concentration of ca. $2 \cdot 10^{18} \text{ cm}^{-3}$. The multiplication coefficient is low, below 200, and it is nearly independent of the compensation impurities for percentages below 0.2 %, and it increases to value up to 10^4 and above in highly compensated boron-doped diamond. The decrease of the multiplication coefficient is attributed to the increase in the number of the carrier at room temperature with the steep decrease of the activation energy above $2 \cdot 10^{18} \text{ cm}^{-3}$ (see **Figure 3**). To our knowledge, there are no available measurements of the carrier multiplication coefficient in boron-doped diamond in the literature. One might estimate the value of the multiplication coefficient based on the ratio of the reported room-temperature carrier concentration determined by Hall effect characterization and acceptor concentration or the boron concentration determined from temperature dependent Hall effect characterization and secondary ions mass spectrometry (SIMS), respectively. The multiplication coefficient determined from the data available in the literature are compared to theoretical room temperature multiplication coefficient on **Figure 2**. These data points, that span over three decades, are within the range of theoretical multiplication coefficient. This figure also indicates that most of the boron-doped diamond layers have a compensation larger than 1 %. On this

figure is also reported the current multiplication coefficient due to impurity impact ionization avalanche determined from data in ref. [1]. Here, we assume the current multiplication coefficient is comparable to the carrier concentration multiplication coefficient as the two current values are measured, on the S-shaped I-V curve, at the same voltage, i.e., same field. This calculated value is consistent with the theoretical value of low compensated and highly boron-doped diamond.

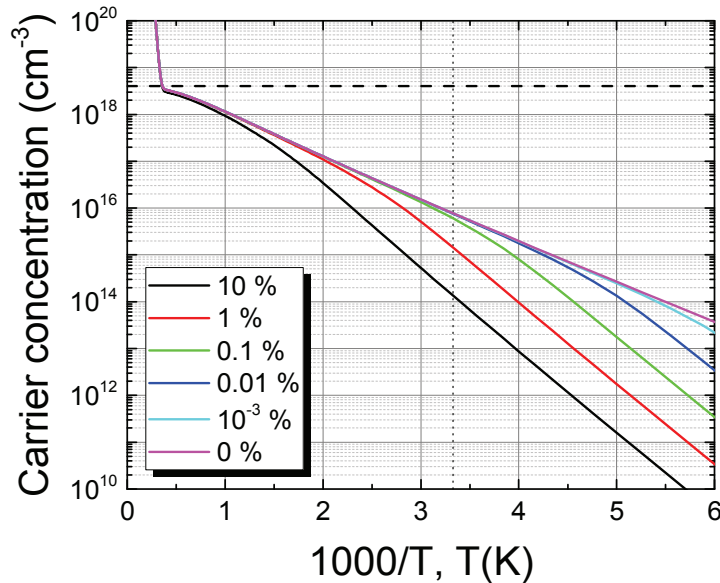


Figure 1 Arrhenius plot of the hole concentration in doped diamond with a boron concentration of $3 \cdot 10^{18} \text{ cm}^{-3}$ for various percentages of compensation impurities

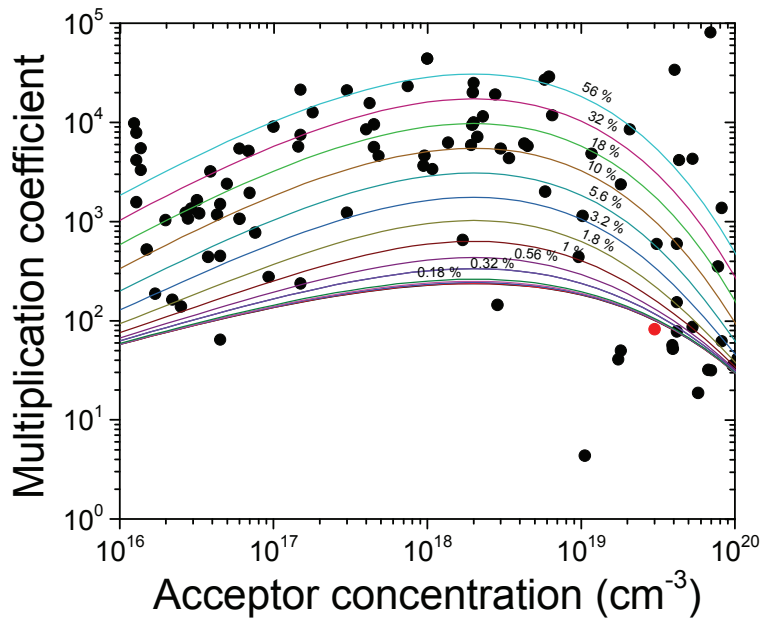


Figure 2 Room temperature carrier concentration multiplication coefficient for various boron concentration and compensation impurities percentages (from 0.01 % to 56 %) and its comparison with acceptor to carrier concentration ratios calculated from data available from the literature (black points) [5-17] and the current multiplication factor (red point) due to impurity impact ionization avalanche in boron-doped diamond determined from ref. [1]

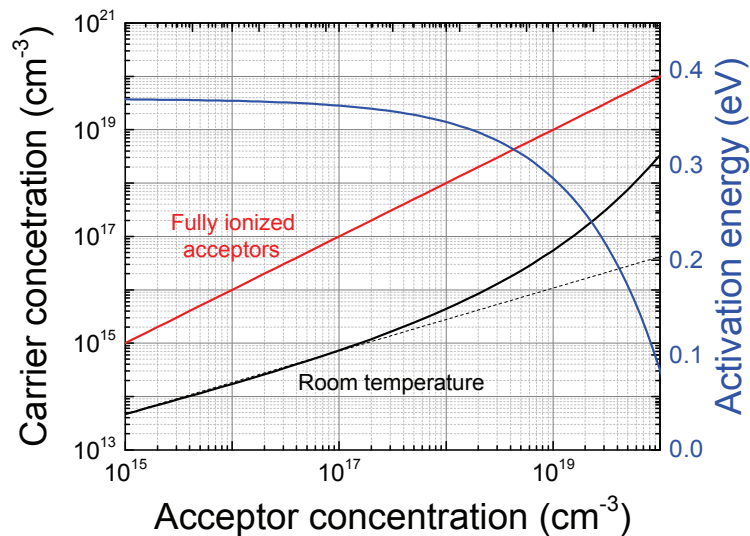


Figure 3 Comparison of the room temperature carrier concentration and the fully ionized acceptor carrier concentration as a function of the acceptor concentration in low compensated boron-doped diamond and variation of the modeled activation energy as a function of the acceptor concentration. Dotted line displays hypothetical carrier concentrations corresponding to the boron activation energy independent of acceptor concentration.

4. CONCLUSION

The theoretical room-temperature hole concentration of boron-doped diamond has been calculated for various acceptor concentration and compensation ratio by solving numerically the charge neutrality equation within the Boltzmann approximation of the Fermi-Dirac statistic and assuming a variation of the activation energy of the dopant in a $-1/3$ power function. These values were used to determine theoretical carrier concentration multiplication coefficients. The multiplication coefficient is the largest for an acceptor concentration of ca. $2 \cdot 10^{18} \text{ cm}^{-3}$ and it increases with the compensation above 0.2 %. These theoretical values are consistent with 1- the ratio of the carrier concentration at room temperature and the acceptor concentration available in the literature and 2- the current multiplication coefficient due to impurity impact ionization avalanche in boron-doped diamond.

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