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Hole states in diamond p-delta-doped field effect transistors

J. C. Martínez-Orozco[1], **I. Rodríguez-Vargas**[1], **M. E. Mora-Ramos**[2]

[1] Unidad Académica de Física, Universidad Autónoma de Zacatecas, Calzada Solidaridad Esquina con Paseo la Bufa S/N, CP 98060 Zacatecas, ZAC., Mexico
[2] Facultad de Ciencias, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa, CP 62209 Cuernavaca, MOR., México

E-mail: `jcmover@correo.unam.mx`

Abstract. The p-delta-doping in diamond allows to create high density two-dimensional hole gases. This technique has already been applied in the design and fabrication of diamond-based field effect transistors. Consequently, the knowledge of the electronic structure is of significant importance to understand the transport properties of diamond p-delta-doped systems. In this work the hole subbands of diamond p-type delta-doped quantum wells are studied within the framework of a local-density Thomas-Fermi-based approach for the band bending profile. The calculation incorporates an independent three-hole-band scheme and considers the effects of the contact potential, the delta-channel to contact distance, and the ionized impurity density.

1. Introduction

Diamond has revealed as a very promising semiconductor material. As very attractive properties, CVD diamond presents unusually high electron and hole mobilities, thermal conductivity and breakdown electric field. This makes it specially suitable for applications in high temperature, high voltage, high frequency and high power electronics [1]. Delta doping techniques have been used to create two-dimensional conductive channels with a high density of charge carriers. Delta-doped quantum wells (DDQW) have associated two-dimensional electron and hole gases provided the type of doping. In the case of p-delta-doping in diamond, the typical situation is the use of boron as the acceptor dopant. Doping concentrations are above 10^{20} cm^{-3}, allowing two-dimensional sheet carrier densities exceeding 10^{13} cm^{-2} [2]. The properties of the two-dimensional hole gas (2DHG) in p-type DDQW have been theoretically investigated in previous works [3, 4, 5].

On the other hand, the interest in diamond p-type delta-doped systems, from the experimental point of view, has been focused in the design and fabrication of electronic devices, mainly Field Effect Transistors (FET). Among these it is the δ-channel JFET with a boron/nitrogen junction [6, 7, 8].

In this article we are going to present the results of a preliminary investigation about the main features of the hole level spectrum in a boron δ-doped diamond FET. To do such a study we use a simplified description of the heavy, light and split-off valence band profiles in the system. This approach uses the so-called depletion approximation to deal with the contact potential barrier and the adjacent uniformly doped region. The potential function associated with the valence
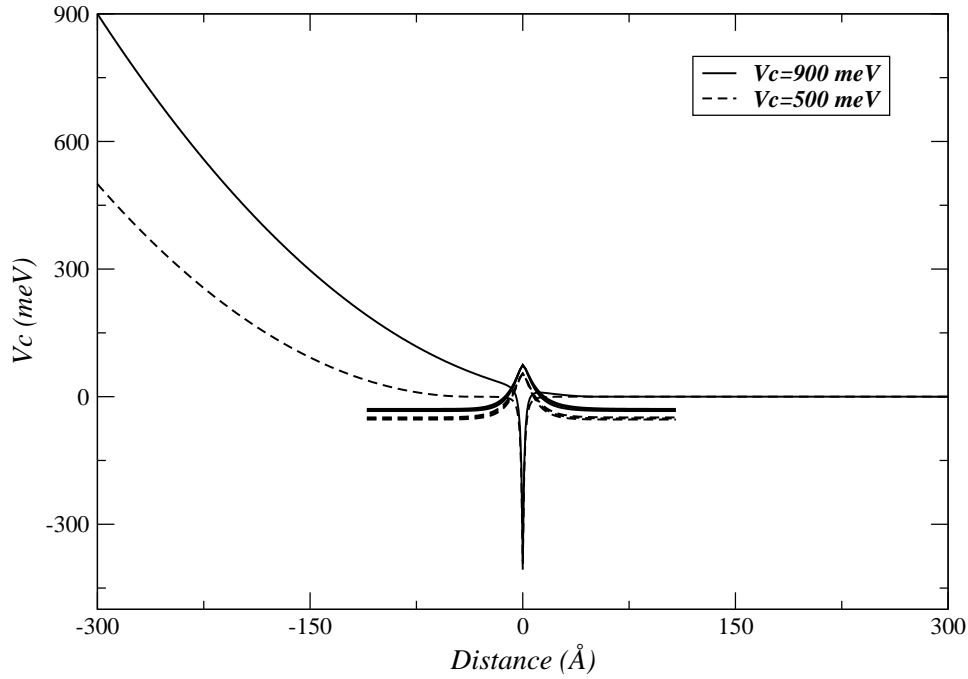
Figure 1. Potential profile and hole wave function for a p-type δ-doped FET in diamond. The two dimensional hole gas in this case is $p_{2D} = 5.0 \times 10^{14}$ cm^{-2}. In this figure the dashed lines correspond to the case of $V_c = 500$ meV and the solid one to $V_c = 900$ meV.

band warping is derived along the lines of the Thomas-Fermi theory [4]. In this approximation, Hartree contributions are explicitly included in the analytic expression for $V(z)$.

2. Model and results

The expression for the Thomas-Fermi potential associated to the delta-like ionized acceptor layer is [9]:

$$V_{TF}(z) - E_F = -\frac{\alpha^2}{(\alpha\,|z - l_d| + z_0)^4}.$$ (1)

Here it is assumed to be in the low temperature limit. l_d is the distance between the delta-channel and the contact barrier. Heavy, light and split-off hole bands are considered uncoupled. This constitutes a fairly good description of the hole dynamics at $\mathbf{k} = \mathbf{0}$. Atomic units are used throughout, referred to an effective Bohr radius $a_0^* = \varepsilon\hbar^2/(e^2 m_{hh})$, and to an effective Rydberg $R_y^* = e^2/(2\varepsilon a_0^*)$. The static dielectric constant of diamond is taken as $\varepsilon = 5.72$. In the above equation E_F is the Fermi level energy, and $\alpha = 2m_a^{3/2}/15\pi$, with $m_a = \left[1 + (m_{lh}/m_{hh})^{3/2} + (m_{so}/m_{hh})^{3/2}\right]^{2/3}$. m_j $(j = mh, lh, so)$ are the corresponding valence bands effective masses in units of the free electron mass, which are 4.27, 3.66 and 3.94 [10]. Additionally,

$$z_0 = \left(\frac{\alpha^3}{\pi p_{2D}}\right)^{1/5},$$ (2)

where p_{2D} is the two-dimensional hole concentration associated to the plane of ionized impurities.

The potential function of equation (1) must combine with the valence band potential energy expression related with the Schottky barrier at the metallic contact. For this, we propose the following modification of the depletion approximation:

$$V_d(z) = 8\pi N_d (z - L_1)^2, \tag{3}$$

where N_d is the three-dimensional density of ionized acceptor impurities in the barrier region. The modified depletion length L_1 is given by:

$$L_1 = \sqrt{L^2 + \frac{1}{8\pi N_d} \frac{\alpha^2}{(\alpha l_d + z_0)^4}}, \tag{4}$$

where

$$L = \sqrt{\frac{V_c}{8\pi N_d}}, \tag{5}$$

is the so-called depletion length associated to the Schottky barrier of contact potential V_c. Finally, the potential function modeling the valence band profile in the system is $V(z) = V_{TF}(z) + V_d(z)$, which is written as,

$$V(z) = 8\pi N_d (z - L_1)^2 \theta(z - L_1) - \frac{\alpha^2}{(\alpha |z - l_d| + z_0)^4} \theta(z - l_d). \tag{6}$$

3. Results and Discussion

Table 1. Energy levels for a diamond δ-FET. The values of energy are given with respect to the well bottom. We also report -in the last column- the width of the depletion region.

V_c (meV)	E_{hh}	E_{lh}	E_{so}	l_p (Å)
100	352.56	357.64	355.25	117.0
200	352.56	357.64	355.25	165.0
300	352.56	357.64	355.25	203.0
400	352.56	357.64	355.25	234.0
500	352.56	357.64	355.25	260.0
600	352.57	357.66	355.26	279.0
700	353.69	358.84	356.41	289.0
800	360.37	365.48	363.08	293.0
900	372.61	377.67	375.29	295.0

The basic input parameters are: background impurities density of $N_d = 1.0 \times 10^{18}$ cm^{-3}, and contact voltage potential V_c from 100 to 900 meV. We locate the p-type δ-doped well 300 Å from the metal-semiconductor contact, and the two-dimensional hole concentration associated with this p-type δ-doped well are $p_{2D} = 5.0 \times 10^{14}$ and $p_{2D} = 7.0 \times 10^{14}$ cm^{-2}.

The first aspect to be analyzed has to do with the way the hole structure is affected as a function of the contact potential. To do this we firstly fix V_c to a very low value, in such a way that we reproduce the results reported for an isolated delta quantum well in ref. [5]. Then we start changing the value of the contact potential and find that for $p_{2D} = 5.0 \times 10^{14}$ cm^{-2}
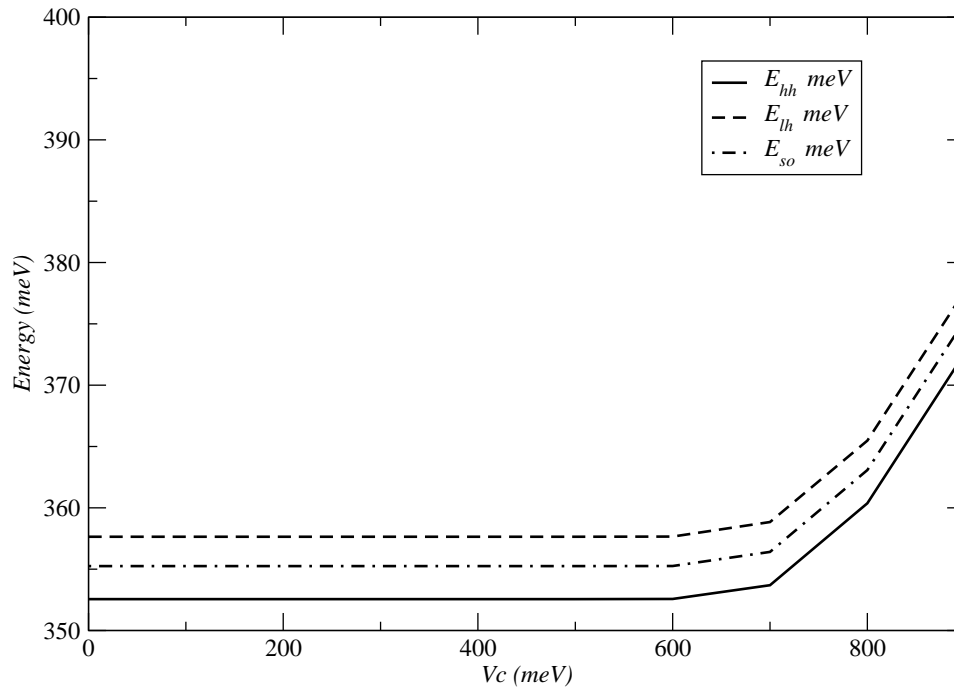
Figure 2. Energy levels as a function of contact potential V_c for an p-type δ-doped FET in diamond.

the well has a depth of 406 meV, and it binds the ground levels of the three hole bands. In figure 1 we present the wave functions calculated for the three ladder of levels. In this figure we present two values of the contact potential, 500 and 900 meV. In table 1 the calculated energies are presented for each of the effective masses m_j $(j = mh, lh, so)$. The energies are reported as functions of V_c. In addition, we give the width of the impurity depletion region, adjacent to the metal-semiconductor contact.

Finally, in figure 2 we show how the energy levels vary as a function of V_c. We find that such levels are practically not affected when $V_c < 600$ meV, and for greater values of this potential the hole level structure is strongly dependent on this parameter.

4. Conclusion

In this work we present the first calculation of the hole level structure in a p-type δ-doped FET in diamond. We find that only three ground states are bound within the well for the set of parameters considered. We also observed regions for which the contact potential significantly affects the electronic energy level structure in the device ($V_c > 600$ meV). Additionally, the proposed model allows us to modify the main parameters of the system and find the optimum values of them in order to achieve the desired features.

Acknowledgments

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