

Simulation of CVD diamond-based high speed near-infrared photodetectors



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ABSTRACT

A near-infrared photodetector on an unbiased p-type CVD diamond Schottky diode is considered and simulated in details. As a diamond-based device, it possesses radiation and chemical endurance and a large hole saturation velocity, determining its potential for high-speed operation. To raise the photodetector sensitivity by thinning the Schottky barrier and thereby increasing its tunneling transparency for holes an alternative to the high homogeneous depletion layer doping is investigated. It consists in the division of the depletion layer into two parts: the thick low-doped part and the highly-doped part (a delta-layer), placed at the depletion layer interface with a metal. It is shown that such doping profile is more advantaged than a high homogeneous doping as it allows to decrease the speed-limiting device capacitance by more than 5 times while maintaining the same device sensitivity.

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1. Introduction

It is commonly accepted that high pressure high temperature (HPHT) and chemically vapor deposited (CVD) diamond can be employed for the fabrication of ultraviolet and soft X-ray photodetectors [1,2], and other X-ray devices [3] and particle detectors [4–6]. Its use as a photodetecting material in the telecommunication near-infrared range is in principle possible due to the formation of impurity bands in its bandgap [7], but, thanks to the difficulty to control and reproduce these bands parameters, has not get much attention.

Nevertheless, there is another way to create a CVD diamond-based near-infrared photodetector. On the analogy with conventional semiconductor optoelectronics [8], it consists in employing Schottky diode structures in which radiation is absorbed not due to interband excitation in CVD diamond, but due to phonon-assisted intraband transitions in the conductivity band of an adjacent metal. The working frequencies of such devices are determined not by the CVD diamond bandgap energy, but by the difference between the Schottky barrier top and the chemical potential (in the hole energy representation). The value of this difference for common metals depends on the metal and CVD diamond surface treatment and can lie close to the telecommunication near-infrared region [9]. The advantages of CVD diamond-based near-infrared Schottky diode photodetectors are attributed to ultrahigh carrier mobility and radiation and chemical endurance of CVD diamond [10], which make their

speed and reliability significantly higher than those of analogous devices based on common semiconductors. These devices can have watt-ampere sensitivities and response times up to 1 A/W and several tens of picoseconds respectively [11–13] (though these record characteristics are not combined in a single device).

The present work is devoted to a theoretical consideration of a CVD diamond-based near-infrared Schottky diode photodetector. As the difference between the Schottky barrier top and the chemical potential tends to lie in the visible region for common metals [14], to operate such a device in the telecommunication near-infrared range we propose to use the modulation doping technic analogous to that employed in the case of common semiconductors (please see [15] and references therein). It consists in fabrication of a low doped CVD diamond film with a highly doped delta-layer in the vicinity of the film interface with a metal. This allows to thin the Schottky barrier upper part and make it transparent for tunneling carriers and, in the same time, to minimize the speed-limiting device capacitance. As a result, a sufficient photocurrent even in the case when the photon energy is smaller than the difference between the Schottky barrier top and the chemical potential can be achieved. All of these make it possible to operate a high-barrier CVD diamond-based Schottky diode photodetector in the telecommunication near-infrared range in a high-speed mode.

2. Mathematical model

In our model of a CVD diamond-based near-infrared Schottky diode photodetector we consider a p-type CVD diamond doped by boron, the shallowest diamond dopant. The boron activation energy

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decrease with the growth of its density (in the density range when the acceptor miniband is not formed yet [16]) is approximated by an empirical formula [17] $E_a = E_{a0} - aN_B^{1/3}$. Here $E_{a0} = 0.37$ eV is the boron low density activation energy [18], N_B – the boron density in cm^{-3} , and $a = 10^{-7}$ eV·cm – a constant calculated from the condition that the theoretically and experimentally [19] found bulk hole densities coincide.

The temperature T is set to the room value (300 K) as the most important for possible applications. The CVD diamond static dielectric constant ϵ is assumed to be 5.7 [18]. The spin-orbit splitting energy, E_{so} , is 6 meV [18]. For the dependence of the energies of holes on their quasiwave vectors we assume the isotropic model with the heavy, light, and split-off hole effective masses equal to $m_{hh} = 0.427m$, $m_{lh} = 0.366m$, and $m_{so} = 0.394m$ respectively, where m is the free electron mass [20]. This assumption and the chosen values of the hole effective masses are usual for simulations of CVD diamond [21–25].

We suggest to use chromium as a metal for a CVD diamond-based near-infrared Schottky diode photodetector. This choice is accounted for by the works [9], [14], which show that chromium Schottky contact with CVD diamond has one of the smallest difference E_m between the Schottky barrier top and the chemical potential (in the hole energy representation) close to 1 eV. Because the working photon energies of the considered type of Schottky diode photodetectors are of order and higher than this difference, chromium seems to be one of the most suitable metals for the fabrication of the proposed CVD diamond-based near-infrared Schottky diode photodetector. As the Schottky barrier height in the CVD diamond, E_b , depends on the chromium and diamond surface treatment, we take for it a value of 1 eV, which is characteristic for this couple of materials [9].

Let us choose the additive constant in the electrical potential ϕ so that the latter approaches zero beside the depletion layer, i.e. at $x=l$, where x is the space coordinate along the axis orthogonal to the CVD diamond-metal interface (Fig. 1) and $l = 1 \mu\text{m}$ is larger (as it follows from the calculations below for all the doping densities used) than the depletion layer thickness.

Let us also count off hole energy E_h downward from the valence band edge at $x=l$. Then, ϕ (and the valence band edge energy,

$E_v = -\phi/e$) distribution at the CVD diamond-metal interface is governed by the one-dimensional Poisson equation.

$$d^2\phi/dx^2 = -4\pi e(p - N_B^-)/\epsilon \quad (1)$$

with boundary conditions $\phi(l) = 0$ and $\phi(0) = E_b/e$. Here e is the value of the elementary charge ($e > 0$), p – the density of holes, N_B^- – the density of negatively charged boron atoms. The last two values depend on the boron atom deposited density, $N_B(x)$, and ϕ according to Fermi–Dirac statistics [27] with the uniform chemical potential μ (counted off from the valence band edge energy at $x=l$ so that $\mu < 0$) determined from the condition of the charge neutrality far from the metal-CVD diamond interface, i.e. from the equation $N_B^-(l) = p(l)$. As the photocurrents considered below are small, they do not influence p and N_B^- significantly, so that Eq. (1) determines ϕ distribution also in the case of nonzero photocurrent densities.

Fermi energies, E_F , of metals which can be used for the CVD diamond Schottky diode photodetectors fabrication are, as a rule, much larger than the room temperature thermal energy $k_B T$, where k_B is the Boltzmann constant. So, for chromium, which is considered here, $E_F \approx 7$ eV [28]. Therefore, in what follows we shall consider the Fermi–Dirac distribution function in the metal a step-like function.

An estimate made on the basis of the Drude model for the chromium dielectric function [27] shows that the intensity of the incident near-infrared radiation with photon energy 1.36 eV used in simulations (please see Section 3) decreases in chromium by e times over a distance of 9 nm. It means that chromium layer 4 (Fig. 1) with a thickness of order 10 nm is practically opaque for the incident radiation and, therefore, prevents its penetration into the CVD diamond. So, we shall neglect the activation of boron atoms in the CVD diamond by the incident radiation and the associated photocurrent induction.

In the metal the incident radiation with a photon energy $\hbar\omega$ excites electrons from energies smaller than the Fermi energy to energies larger than the Fermi energy (the electron energy E_e is counted off upward from the metal conductivity band edge energy E_c). It leads to the creation of holes with energies E_h from μ to $\mu + \hbar\omega - E_{ph}$. Here E_{ph} is the energy of a phonon emitted simultaneously with the electron excitation due to the condition of the electron quasimomentum conservation. As characteristic E_{ph} (determined by the Debye temperature) in chromium is much smaller than $\hbar\omega$ in the near-infrared region [29], in what follows we shall neglect E_{ph} in comparison with $\hbar\omega$. So, the interval of the possible values of E_h is assumed to lie from μ to $\mu + \hbar\omega$. The distribution of E_h in it, η_e , is proportional to the product of the electron densities of states in the metal at energies $E_F + \mu - E_h$ and $E_F + \mu - E_h + \hbar\omega$, i.e. at the energies of the initial and final states of the electron transition. But in the case considered all the values $|\mu|$, E_h and $\hbar\omega$ are much smaller than E_F so that this product is nearly a constant and, therefore, can be ignored when finding the distribution of E_h . Thus, this distribution is uniform and given by the formula.

$$\eta_e = 1/(\hbar\omega). \quad (2)$$

To tunnel from the metal into the CVD diamond layer through the Schottky barrier the photocreated holes must have $E_h > 0$ and a small enough in-plane quasimomentum. The latter condition is due to the fact that in the CVD diamond the hole quasimomentum is $\sqrt{2m_h E_h}$, where m_h is the hole mass. Meanwhile, in the metal the hole quasimomentum is $\sqrt{2m(E_F + \mu - E_h)}$, which is much larger than $\sqrt{2m_h E_h}$. So, due to the in-plane quasimomentum and energy conservation, only holes with in-plane quasimomenta smaller than $\sqrt{2m_h E_h}$ can tunnel from the metal into the CVD diamond layer through the Schottky barrier. Assuming the spherical symmetry in the distribution of the hole quasimomentum directions in the metal, it is easy to show that the ratio of the number of holes which, after tunneling, would have in the CVD diamond layer the orthogonal to the Schottky barrier

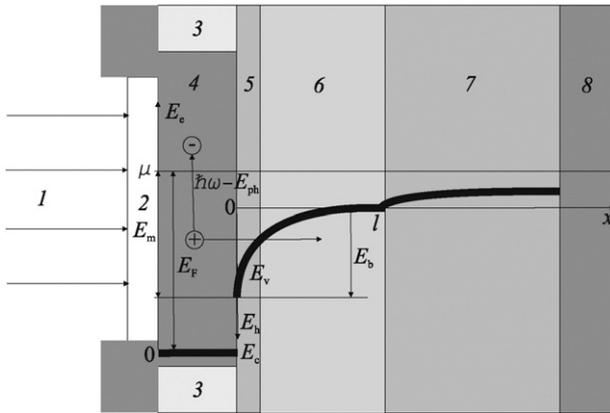


Fig. 1. A scheme of a CVD diamond-based near-infrared Schottky diode photodetector (the layer thicknesses are not to scale): 1 – incident near-infrared radiation, 2 – anti-reflection coating [8], 3 – isolating SiO_2 layers [8], 4 – a thin (with a thickness of order 10 nm) chromium layer [8], 5 – a CVD diamond highly-doped delta-layer (the optimal doping density and thickness are determined below), 6 – a low-doped (the optimal doping density is determined below) CVD diamond layer (the total thickness of layers 5 and 6 is l), 7 – a highly (on the order of 10^{20} cm^{-3}) boron doped $100 \mu\text{m}$ -thick CVD diamond layer [26] (a thinned substrate needed to maintain the mechanical stability of otherwise too thin a structure), 8 – a Ti/Pt/Au ohmic contact [26]. All the other notations are explained in detail in the text below: μ – the chemical potential, E_m – the difference between the Schottky barrier top and the chemical potential in the hole energy representation, E_F – the metal Fermi energy, $\hbar\omega$ – the incident radiation photon energy, E_{ph} – the phonon energy, E_c – the metal conductivity band edge energy, E_v – the valence band edge energy, E_b – the Schottky barrier height in the CVD diamond. The electron energy E_e is counted off upward from E_c , whereas the hole energy E_h is counted off downward from E_v at $x=l$.

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