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Approximate Solution to Kinetic Equation for Simulation of a Perfect CVD Diamond Schottky Diode with a Steep Forward Current-Voltage Characteristic

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Abstract

Two time scales in relaxation of charge carriers in the chemically vapor deposited (CVD) diamond (fast relaxation to equilibrium distribution when their kinetic energies are larger than the optical phonon energy and slow relaxation in the opposite case) and the large (in comparison with the room-temperature thermal energy) optical phonon energy lead to a situation when neither diffusion nor diode theory for the calculation of the perfect CVD diamond Schottky diode current-voltage characteristic (CVC) is valid. So, the kinetic equation approach to this characteristic simulation is considered. The above mentioned existence of two time scales of relaxation processes allows to obtain an approximate solution to this equation. It results in the ideality factor for the perfect CVD diamond Schottky diode CVC significantly smaller than unity. On the other hand, CVCs of perfect Schottky diodes on usual semiconductors, for which either diffusion or diode theory is valid, are described by Shockley's formula, i.e. by the ideality factor equal to unity. It means that perfect Schottky diodes on the CVD diamond have a significantly steeper forward branch of the CVC than perfect devices of such a type on usual semiconductors.

Keywords: CVD Diamond, Kinetic Equation, Schottky Diode Current-Voltage Characteristic

1. Introduction

Chemically vapor deposited (CVD) diamond has unique characteristics (among those are very high charge carrier mobilities, saturation velocities, breakdown electric field, thermal conductivity and optical transparency in a large wavelength range from ultraviolet to far-infrared domain, radiation and chemical endurance, a small thermal expansion coefficient and others) which make it a very promising substitute for usual semiconductors when creating high-power and high-frequency electronic devices capable of operation in harsh environment [1, 2, 3]. The base of CVD diamond electronics could be p-n junctions as it takes place in ordinary semiconductor electronics. Unfortunately, due to the difficulty of incorporation of p- and n-dopants of the CVD diamond into its lattice and their high activation energies, the growth of sufficiently conductive p- and n-CVD diamond layers while maintaining their high crystalline quality needed for electronics applications is by no means an easy task [4]. Because boron, the shallowest CVD diamond p-dopant [5], has significantly lower activation energy than phosphorous, one of the most suitable CVD diamond n-dopants [6, 7], and comparatively easily incorporates into diamond lattice, the technology of the creation of p-type CVD diamond layers with required characteristics is well-established now [8]. But the growth of n-type CVD diamond layers with suitable parameters is a much more difficult task [4].

Therefore, a lot of attention has been paid to the creation of p-CVD diamond–metal junctions (i.e. Schottky diodes), which can to some extent substitute for p-n CVD diamond junctions. Such devices or their prototypes were successfully realized [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24] and showed unique parameters [25]. In this regard an important task is the simulation of their current-voltage characteristics (CVCs). Its fulfilment is obstructed by the fact that for Schottky diodes on p-type CVD diamond it can be done by neither diffusion [26], nor diode [27] theories.

Indeed, the first theory requires that the hole density change significantly at distances much larger than the hole free pass length. When holes form a nongenerate gas (as it takes place at comparatively low boron doping densities considered below), at zero external bias this means the fulfillment of condition

$$eu_{\mathrm{c}}l_{\mathrm{f}}/(k_{\mathrm{B}}Tl) \ll 1. \tag{1}$$

Here e is the elementary charge ($e > 0$), u_{c} – the contact potential difference, l_{f} – the hole free pass length, k_{B} – Boltzmann's constant, T – temperature, l

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– the depletion layer thickness. When the hole energy in diamond is at least several times larger than the optical phonon energy, $\hbar\omega_{\mathrm{o}}$, hole scattering by optical phonons dominates that by acoustic phonons and ionized boron atoms for comparatively low boron doping densities considered below [28, 29]. On the other hand, the hole scattering by acoustic phonons and ionized boron atoms for comparatively low boron doping densities considered below is sufficiently weak. In result, l_{f} can be estimated as $l\hbar\omega_{\mathrm{o}}/(eu_{\mathrm{c}})$, i.e. as a length (counted off from the CVD diamond–metal interface) at which, due to the acceleration in the depletion layer electric field, the kinetic energy of a hole (whose kinetic energy at the CVD diamond–metal interface is of order the thermal energy $k_{\mathrm{B}}T$, which is much smaller than $\hbar\omega_{\mathrm{o}}$ at room temperature [5]) becomes of order $\hbar\omega_{\mathrm{o}}$. So, the left hand side of (1) equals $\hbar\omega_{\mathrm{o}}/(k_{\mathrm{B}}T)$. This value is much larger than unity and, therefore, condition of the diffusion theory validity (1) is not satisfied.

The diode theory requires that at zero external bias condition

$$l_{\mathrm{f}}/l \gg 1 \tag{2}$$

is fulfilled. According to what was said above, $l_{\mathrm{f}}/l \sim \hbar\omega_{\mathrm{o}}/(eu_{\mathrm{c}})$. As for usual metals $eu_{\mathrm{c}} \gg \hbar\omega_{\mathrm{o}}$, condition of the validity of the diode theory (2) is not satisfied either.

Thus, the simulation of the CVCs of Schottky diodes on CVD diamond requires the numerical solution to the system of kinetic and Poisson's equations describing hole motion in inhomogeneous electrical field of the depletion layer. But such an approach is computationally difficult as one needs to turn over all physically possible hole distribution functions at the CVD diamond–metal interface to find the one which, according to the solution to the system of kinetic and Poisson's equations, leads to the known asymptotic hole distribution function and field in the CVD diamond beyond the depletion layer. This can be realized by means of powerful computer systems only.

But, due to the above mentioned sharp increase of the scattering rate of a hole as its energy exceeds the optical phonon energy $\hbar\omega_{\mathrm{o}}$, kinetic equation has an approximate solution. To find it also requires computer calculations, but much simpler than those to obtain the exact solution to kinetic equation. Being coupled to the solution to Poisson's equation, this approximate solution allows to find the CVCs of perfect (i.e. free from the drawbacks deteriorating their performance and considered in the Results and Discussion Section) Schottky diodes on CVD diamond. It shows that they are characterized by

the ideality factor significantly smaller than unity. On the other hand, CVCs of perfect Schottky diodes on usual semiconductors for which either the diffusion or diode theory is valid are described by Shockley's formula, i.e. by the ideality factor equal to unity. It means that perfect Schottky diodes on CVD diamond are characterized by a significantly more rapid growth of the forward current with the increase of the forward bias than perfect Schottky diodes on usual semiconductors. This fact may present an important advantage of Schottky diodes on the CVD diamond over such devices on usual semiconductors in electronics applications.

The present article is devoted to the detailed consideration of the approximate kinetic equation solution method for the simulation of the CVCs of perfect Schottky diodes on the CVD diamond.

2. The Method of Approximate Solution to Kinetic Equation

Let us use one-dimensional approach valid when the diode thickness is much smaller than its transversal dimensions along axes y and z in Cartesian's coordinate frame (Fig. 1). So, all the physical quantities will depend on single coordinate x counted off from the CVD diamond–metal interface towards the CVD diamond layer.

Let us denote the coordinate-dependent quasiclassical hole distribution function over quasiwavevectors $\boldsymbol{k}$ in heavy, light and spin-orbit split-off bands by f_{hh}, f_{lh} and f_{so} respectively. Let us choose their norms so that

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} 2 f_{\mathrm{hh,lh,so}} \mathrm{d}k_x \mathrm{d}k_y \mathrm{d}k_z / (2\pi)^3 = n_{\mathrm{hh,lh,so}}, \qquad (3)$$

where $n_{\mathrm{hh,lh,so}}$ are the coordinate-dependent hole densities in the respective bands and factor 2 stands for the band double degeneracy. Distribution functions $f_{\mathrm{hh,lh,so}}$ obey kinetic equation, which in the stationary situation considered here reads as

$$\frac{\hbar k_x}{m_{\mathrm{hh,lh,so}}} \frac{\partial f_{\mathrm{hh,lh,so}}}{\partial x} - \frac{e}{\hbar} \frac{\mathrm{d}\phi}{\mathrm{d}x} \frac{\partial f_{\mathrm{hh,lh,so}}}{\partial k_x} = \mathrm{St}_{\mathrm{hh,lh,so}}, \qquad (4)$$

where $m_{\mathrm{hh,lh,so}}$ are the heavy, light and spin-orbit split-off hole masses respectively, ϕ – the electrostatic potential, and $\mathrm{St}_{\mathrm{hh,lh,so}}$ – the collision integrals in which hole scattering by acoustic and optics phonons and ionized boron atoms are taken into account.
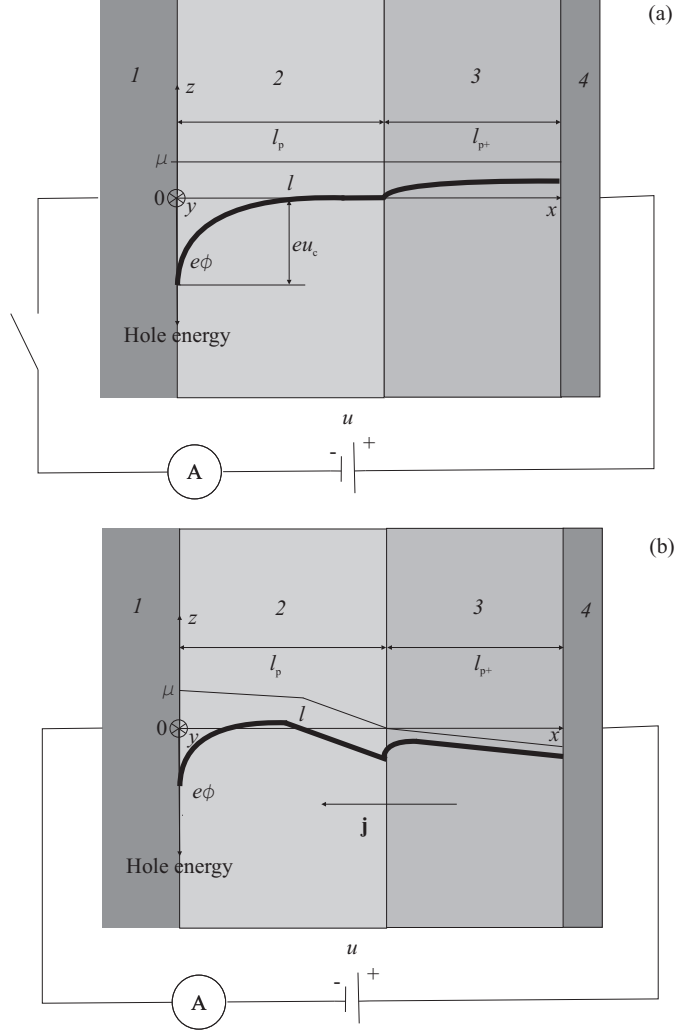
Figure 1: Schematic (not to scale) of the CVD diamond-based Schottky diode: 1 – a metal (chromium) layer, 2 – a low (boron-) doped CVD diamond layer (thickness l_p), 3 – a highly (boron-) doped CVD diamond layer (thickness l_{p^+}), 4 – an ohmic contact. Also shown are the Cartesian coordinate system used in the text, the electrostatic hole energy $e\phi$ (i.e. the valence band edge energy, ϕ – the electrostatic potential), the chemical potential μ coordinate dependence and the contact potential difference u_c. (a) – equilibrium situation (current density $j = 0$), (b) – nonequilibrium situation ($j \neq 0$)

When external bias u is zero (i.e. in equilibrium), $f_{\mathrm{hh,lh,so}}$ are given by Fermi–Dirac's distributions [26] (which nullify St), namely

$$f_{\mathrm{hh,lh}} = \frac{1}{\exp\{[\hbar^2 k^2/(2m_{\mathrm{hh,lh}}) + e\phi - \mu]/(k_{\mathrm{B}}T)\} + 1}, \tag{5}$$

$$f_{\mathrm{so}} = \frac{1}{\exp\{[E_{\mathrm{so}} + \hbar^2 k^2/(2m_{\mathrm{so}}) + e\phi - \mu]/(k_{\mathrm{B}}T)\} + 1}, \tag{6}$$

where E_{so} is the spin-orbit splitting energy, $e\phi$ – the valence band edge energy. In equilibrium the ionized boron atom density, n_{B}^-, is also given by a Fermi–Dirac-like function [26],

$$n_{\mathrm{B}}^- = \frac{n_{\mathrm{B}}}{2\exp[(\mu - e\phi - E_{\mathrm{a}})/(k_{\mathrm{B}}T)] + 1}, \tag{7}$$

where n_{B} is the doping boron density and E_{a} – the boron activation energy dependent on the boron density, $E_{\mathrm{a}} = -(E_{\mathrm{a0}} - \alpha n_{\mathrm{B}}^{1/3})$ [30].

Electrical potential obeys Poisson's equation

$$\mathrm{d}^2\phi/\mathrm{d}x^2 = -4\pi e(n - n_{\mathrm{B}}^-)/\varepsilon \tag{8}$$

with boundary conditions $\phi(0) = u_{\mathrm{c}}$ and $\phi(l) = 0$. Here $n \equiv n_{\mathrm{hh}} + n_{\mathrm{lh}} + n_{\mathrm{so}}$ is the total hole density and ε – the diamond static dielectric constant. The value of the chemical potential is determined from the condition that the charge density is zero at $x = l$, i.e. that $n = n_{\mathrm{B}}^-$ at this point.

When the external bias u is nonzero, current with density $\boldsymbol{j}$ flows through the device. In this nonequilibrium situation the hole distribution functions in the subbands are not given by Fermi–Dirac's formulas. Nevertheless, it is possible to introduce a formal nonequilibrium chemical potential μ, whose coordinate dependence is chosen such, that, after its substitution into Fermi–Dirac's equilibrium formulas (3), (5), and (6), it gives the true coordinate dependence of nonequilibrium hole density $n \equiv n_{\mathrm{hh}} + n_{\mathrm{lh}} + n_{\mathrm{so}}$. Then, as current densities j considered below are rather small, the non-equilibrity does not significantly influence the neutral boron atoms thermal ionization and the reverse process of hole recombination with negatively charged boron atoms. So, at $j \neq 0$ negatively charged boron atoms density n_{B}^- is connected with hole density n by the same relation as at $j = 0$. But at $j = 0$ this relation is given by formula (7), where μ is expressed as a function of $n \equiv n_{\mathrm{hh}} + n_{\mathrm{lh}} + n_{\mathrm{so}}$ by formulas 3), (5), and (6). Then, at $j \neq 0$ value n_{B}^- is still given by formula (7) with the above-introduced formal nonequilibrium chemical potential μ.

Beyond the depletion layer μ has to be a linear function of x with a slope $e\,\mathrm{d}\phi/\mathrm{d}x$, where $-\mathrm{d}\phi/\mathrm{d}x \equiv E = j\rho$ is the electric field providing the flow of current with density j in the CVD diamond with specific resistance ρ. So, bearing in mind the smoothness of the nonequilibrium chemical potential coordinate dependence at comparatively small current densities considered below, let us approximate this coordinate dependence by linear functions, namely $\mu = \mu_0 - eE(x - l)$ for x larger than the depletion layer thickness l and $\mu = \mu_0 - e\tilde{E}(x - l)$ for $0 < x < l$.

The charge density $e(n - n_{\mathrm{B}}^-)$ being determined by μ, the nonequilibrium electric potential distribution can be found from the solution to Poisson's equation (8) with the following conditions at point $x = l$. First, as far from the metal–CVD diamond interface ϕ has to be a linear function of x with slope $-E$, let us assume that such coordinate dependence of ϕ holds true down to l, so that at $x = l$ one has $\mathrm{d}\phi/\mathrm{d}x = -E$. Second, as ϕ is determined up to an arbitrary additive constant, let us chose the latter so that $\phi(l) = 0$. These are two conditions at point $x = l$ unambiguously determining the solution to Poisson's equation (8).

To find three constants μ_0, $\tilde{E}$ and l left undetermined in the above analysis, let us employ the following considerations. First, the value of μ_0 is chosen from the condition of charge neutrality at point $x = l$, i.e. $n(l) = n_{\mathrm{B}}^-(l)$. Second, let us as usual [27] assume that at the metal–CVD diamond interface the distribution functions of holes with positive quasiwavevector x-components (i.e. of holes, penetrating into the CVD diamond from the metal) remains the same as in equilibrium. So, the hole density, n^+, and the current density, j^+, due to holes with positive quasiwavevector x-components at $x = 0$ are given by formulas

$$n^+ = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{0}^{+\infty} 2(f_{\mathrm{hh}} + f_{\mathrm{lh}} + f_{\mathrm{so}}) \frac{\mathrm{d}k_x \mathrm{d}k_y \mathrm{d}k_z}{(2\pi)^3}, \qquad (9)$$

$$j^+ = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{0}^{+\infty} j_{\boldsymbol{k}}^+ \frac{\mathrm{d}k_x \mathrm{d}k_y \mathrm{d}k_z}{(2\pi)^3}, \qquad (10)$$

where $j_{\boldsymbol{k}}^+ \equiv 2e\hbar k_x (f_{\mathrm{hh}}/m_{\mathrm{hh}} + f_{\mathrm{lh}}/m_{\mathrm{lh}} + f_{\mathrm{so}}/m_{\mathrm{so}})$, distribution functions f_{hh}, f_{lh}, and f_{so} are calculated by equilibrium formulas (5) and (6) with equilibrium μ and $\phi = \phi(0)$.

To find the analogous to n^+ and j^+ values due to holes with negative quasiwavevectors x-components at $x = 0$ (i.e. due to holes going to the metal–CVD diamond interface from the CVD diamond), n^- and j^-, let us

employ the following considerations. Distribution functions of holes with negative quasiwavevectors x-components at the metal–CVD diamond interface for kinetic energies $\hbar^2 k^2 / (2m_{\mathrm{hh,lh,so}})$ larger than the optical phonon energy $\hbar\omega_{\mathrm{o}}$ are given by equilibrium Fermi–Dirac's formulas (5) and (6) with $\mu = \mu(0)$ and $\phi = \phi(0)$ due to a short relaxation time of the hole distributions to the equilibrium ones in this energy range. For smaller kinetic energies hole distribution functions are again given by Fermi–Dirac's formulas (5) and (6), but with μ and ϕ taken not at $x = 0$, but at points $x > 0$ where the hole kinetic energies $\hbar^2 k^2 / (2m_{\mathrm{hh,lh,so}}) + e[\phi(0) - \phi(x)]$ (increased in comparison with their values $\hbar^2 k^2 / (2m_{\mathrm{hh,lh,so}})$ at $x = 0$ due to acceleration in the depletion layer electric field) are equal to the optical phonon energy $\hbar\omega_{\mathrm{o}}$. This is due to the facts that, first, at any $x \geq 0$ the distribution functions of holes with kinetic energies larger than $\hbar\omega_{\mathrm{o}}$, due to a short relaxation time of the hole distributions to the equilibrium ones in this energy range, are given by equilibrium Fermi–Dirac's formulas (5) and (6) with $\mu = \mu(x)$ and $\phi = \phi(x)$. Second, due to a comparatively week scattering of holes by acoustic phonons [29] and ionized boron atoms (at the moderate boron doping density considered below), they travel distance x without collisions[1], so that, according to Liouville's theorem, their distribution functions at $x = 0$ are the same as at $x \neq 0$. This allows to find the distribution functions of holes with negative quasiwavevectors x-components at the metal–CVD diamond interface for any hole kinetic energy and use them to calculate n^- and j^- by formulas, analogous to (9) and (10), but in which the integration with respect to k_x is from $-\infty$ to 0.

So found n^- and j^- are dependent on $\tilde{E}$ and l as on parameters. These parameters can be found from the conditions that $n^+ + n^-$ is equal to the hole density n, obtained by Fermi–Dirac's formulas with $\mu(0)$ and $\phi(0)$, and $j^+ + j^-$ is equal to $j_x = -j$.

Then, the potential drop on the CVD diamond Schottky diode can be calculated from the solution to Poisson's equation (8) as $\phi(0)$ (remembering that $\phi(l) = 0$ because of the above mentioned choice of the arbitrary constant in ϕ) plus the potential drop across the distance from l to the ohmic contact (layer *4* in Fig. 1). In what follows we shall neglect the potential drop across the ohmic contact itself as it can be made to have rather a low specific resistance of order $10^{-5} \div 10^{-6}$ $\Omega{\cdot}\mathrm{cm}^2$ [8] so that even for the highest current

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[1]The estimate, corroborating this statement, is in the next section.

density used below (of order 10^{-1} A/cm^2) this drop is smaller than 10^{-6} V.

3. Results and Discussion

To apply the above proposed method of the calculation of CVCs of perfect Schottky diodes on the CVD diamond let us consider a typical device of such a type [16]. It consists of a layer with thickness $l_{\mathrm{p}} = 1.6$ μm (layer 2 in Fig. 1) comparatively low ($n_{\mathrm{B}} = 5 \cdot 10^{16}$ cm^{-3}) boron-doped to increase the breakdown diode voltage which is proportional to $n_{\mathrm{B}}^{-3/4}$ [25]. This layer is on the top of a highly ($n_{\mathrm{B}} = 10^{20}$ cm^{-3}) boron-doped contact layer with thickness $l_{\mathrm{p+}} = 2$ μm (layer 3 in Fig. 1).

For the metal forming Schottky's contact with the low boron-doped CVD diamond layer 2 let us choose chromium (layer 1 in Fig. 1). This choice is accounted for by the works [25, 31], which show that chromium Schottky contact with the CVD diamond has one of the smallest Schottky contact potential difference u_{c} and, therefore, one of the smallest turn-on voltage. The actual value of the latter depends on the surface treatment of a particular CVD diamond sample. Therefore, let us take for u_{c} a value of 1.05 V, which is characteristic for this couple of materials [25].

Let us use for the boron low density activation energy E_{a0} a value of 0.37 eV [5] and for α – a value of 10^{-7} eV·cm, calculated from the condition that the theoretically and experimentally [32] found bulk hole densities at one and the same n_{B} 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 [5]. The spin-orbit splitting energy E_{so} is 6 meV, the characteristic value of the optical phonon energy $\hbar\omega_{\mathrm{o}}$ is 165 meV [5]. For the dependence of the energies of holes on their quasiwavevectors we assume the isotropic model with the heavy, light, and spin-orbit split-off hole effective masses equal to $m_{\mathrm{hh}} = 0.427m$, $m_{\mathrm{lh}} = 0.366m$, and $m_{\mathrm{so}} = 0.394m$ respectively, where m is the free electron mass [33]. This assumption and the chosen values of the hole effective masses are usual for the simulations of CVD diamond-based electronic devices [34, 35, 36].

The external bias u (the forward external bias corresponds to $u < 0$ and the forward current density – to $j_x < 0$) is calculated by the substraction of the potential drop in the equilibrium situation ($j = 0$), $u_{\mathrm{c}} + u_{\mathrm{p\text{-}p+}}$, where $u_{\mathrm{p\text{-}p+}}$ is the potential drop across the p-p$^+$ junction of the low doped layer 2 and the highly doped contact layer 3 (Fig. 1), from the potential drop in the nonequilibrium situation ($j \neq 0$), $\phi(0) - \phi(l) - j(l_{\mathrm{p}} - l)/\rho_{\mathrm{p}} + u_{\mathrm{p\text{-}p+}} - jl_{\mathrm{p+}}/\rho_{\mathrm{p+}}$,
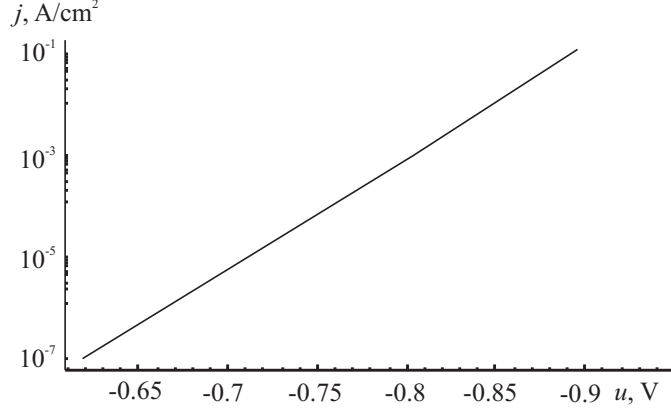
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Figure 2: The current-voltage characteristic of the perfect chromium Schottky diode on the CVD diamond calculated by the proposed method for $10^{-7} \mathrm{A/cm^2} < j < 10^{-1}$ $\mathrm{A/cm^2}$.

where, according to what was said above, $\phi(l) = 0$, ρ_p and $\rho_\mathrm{p^+}$ are the specific resistance of the boron-doped CVD diamond in layer *2* and layer *3* (Fig. 1) respectively taken from the experimental results of [32]. Here we neglect the influence of the current on the value of $u_\mathrm{p\text{-}p^+}$ as, according to the estimates, for the used below comparatively low $j \lesssim 10^{-1}$ $\mathrm{A/cm^2}$ this influence results in the shifts of $u_\mathrm{p\text{-}p^+}$, whose absolute values is much smaller than u_c and, therefore, characteristic absolute values of u.

The obtained dependence of the current density j on the external bias u is shown in Fig. 2. Numerical analysis shows that it cannot be approximated by Shockley's formula [37]

$$j = j_0 \{ \exp[-eu/(k_\mathrm{B}T)] - 1 \} \qquad (11)$$

(to which both the diffusion [26] and diode [27] theories lead) with any choice of the value of j_0. This fact is quite understandable because, as was mentioned in Introduction, neither diffusion, nor diode theory is valid for the description of the CVC of a perfect Schottky diode on the CVD diamond.

The CVC of the perfect chromium Schottky diode on the CVD diamond shown in Fig. 2 can be approximated by Shockley's formula (11) only after the introduction of an ideality factor n [37] in the denominator of the exponent power in it. This approximation is achieved for $n \simeq 0.77$ and $j_0 \simeq 3.3 \cdot 10^{-21}$ $\mathrm{A/cm^2}$. On the other hand, for the Schottky barrier height

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1.3 eV (equal to $eu_c - \mu$, $\mu < 0$) used in the present simulation the experimental CVC of the Schottky diode on the CVD diamond is approximated by Shockley's formula (11) with ideality factor $n \simeq 4.06$ in the denominator of the exponent power in it and $j_0 \simeq 1.13 \cdot 10^{-15}$ A/cm^2 [18]. That n and j_0 calculated in the present study are significantly smaller than those obtained by the approximation of the experimental CVC of the Schottky diode on the CVD diamond [18] is accounted for by the following. The model developed in the present article applies to a perfect Schottky diode on the CVD diamond and does not take into account such imperfection effects as leakage current [38, 39], inhomogeneous Schottky barrier height along the metal–CVD diamond interface [18], the formation of an interfacial layer on this interface [14] and others taking place in a real imperfect device of such a type. These factors lead to a significant deviation of the calculated CVC of a perfect chromium Schottky diode on the CVD diamond from the experimental ones. So, the proposed method can be applied to a real device only after taking into account all the above mentioned effects leading to its imperfection.

Nevertheless, it is important to stress that the calculated ideality factor of a perfect chromium Schottky diode on CVD diamond $n \simeq 0.77$ is significantly smaller than unity. On the other hand, CVCs of perfect Schottky diodes on usual semiconductors for which either diffusion or diode theory is valid are described by Shockley's formula (11), which implies ideality factor $n = 1$. It means that in perfect Schottky diodes on the CVD diamond forward current grows much more quickly with the increase of the forward bias than it takes place in perfect Schottky diodes on usual semiconductors. This means that potentially (i.e. after eliminating the above mentioned causes of their imperfection) Schottky diodes on CVD diamond are characterized by a much more rapid forward current – forward bias dependence than Schottky diodes on usual semiconductors, which represents their important advantage over the latter.

Figure 2 does not show the reverse branch of the CVC of the perfect chromium Schottky diode on the CVD diamond. This is because at the considered parameters the maximal value of the reverse current density (not regarding the breakdown processes which are out of the scope of the present study) $j^+ \simeq 1.6 \cdot 10^{-15}$ A/cm^2. This value is extremely low and, probably, lies down the detection limit.

Now, let us make estimates, corroborating the previous section statements. The characteristic electric field strength at the CVD diamond–metal interface approximates to $(u_c + u)/l(u)$. Then, the distance (counted off from

the metal surface) at which the hole kinetic energy becomes equal to optical phonon energy $\hbar\omega_o$ is smaller than $l_f(u) = l(u)\hbar\omega_o/[e(u_c + u)]$, i.e. smaller than the value of this distance for a hole with zero kinetic energy at $x = 0$. Numerical analysis shows that for the external bias range used in Fig. 2 the depletion layer thickness $l(u) \gtrsim 100$ nm and, therefore, $l_f(u) \lesssim 100$ nm with $l_f(0) \sim 20$ nm. Then, practically for all used u value $l_f(u)$ is smaller than the hole free path length between scattering events by acoustic phonons (which is of order 100 nm [29]) and ionized boron atoms (which is also of order 100 nm as obtained by using Conwell–Weisskopf's formula [40] with ionized boron density n_B^- calculated for the boron atom density $n_B = 5 \cdot 10^{16}$ cm^{-3} in the low-doped layer 2 in Fig. 1). On the other hand, the free path length of a hole with kinetic energy $2\hbar\omega_o$ is of order 0.4 nm [29] (i.e. of order the diamond lattice constant [5]) and, therefore, much smaller than all the above mentioned distances. Then, when the hole kinetic energy becomes of order $\hbar\omega_o$ at distance $l_f(u)$, it practically simultaneously emits an optical phonon, i.e. undergoes a scattering event. In the same time, it travels distance $l_f(u)$ without collisions. So, indeed, as was assumed in the previous sections, $l_f(u)$ represents the hole free path length with respect to all collision processes.

4. Conclusion

In conclusion, it is shown that though the forward branch of the current-voltage characteristic of a perfect CVD diamond based Schottky diode cannot be simulated by the usual diffusion or diode approaches, it can be calculated by means of the proposed method based on the approximate solution to kinetic equation. This solution employs characteristic for the CVD diamond large difference in the charge carrier relaxation rates when their energies are smaller or larger than the optical phonon energy. In results it is shown that in perfect CVD diamond-based Schottky diodes forward current grows with the increase of forward bias much more rapidly than in perfect Schottky diodes on usual semiconductors for which either diffusion or diode theory is valid. It means that CVD diamond-based Schottky diodes have an important potential (i.e. realized after eliminating the causes of their imperfection) advantage over analogous devices on usual semiconductors. The proposed method (after taking into account imperfection factors pertaining to a concrete CVD diamond-based Schottky diode) can be used for finding the CVD diamond parameters (depletion layer doping profile, surface treatment, etc.) and metal type required to provide Schottky diode characteristics needed for

a particular application. This analysis is a subject of future work.

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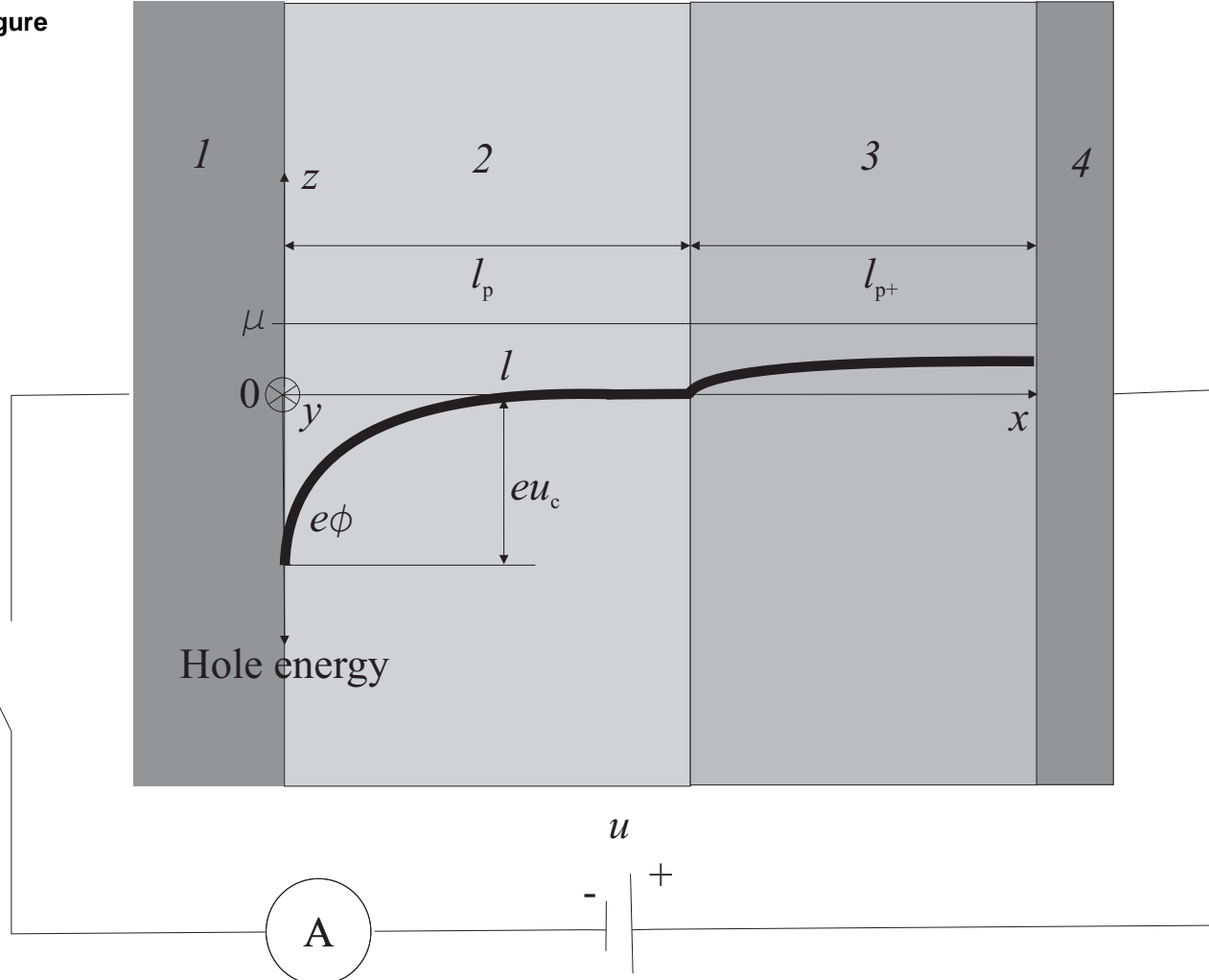
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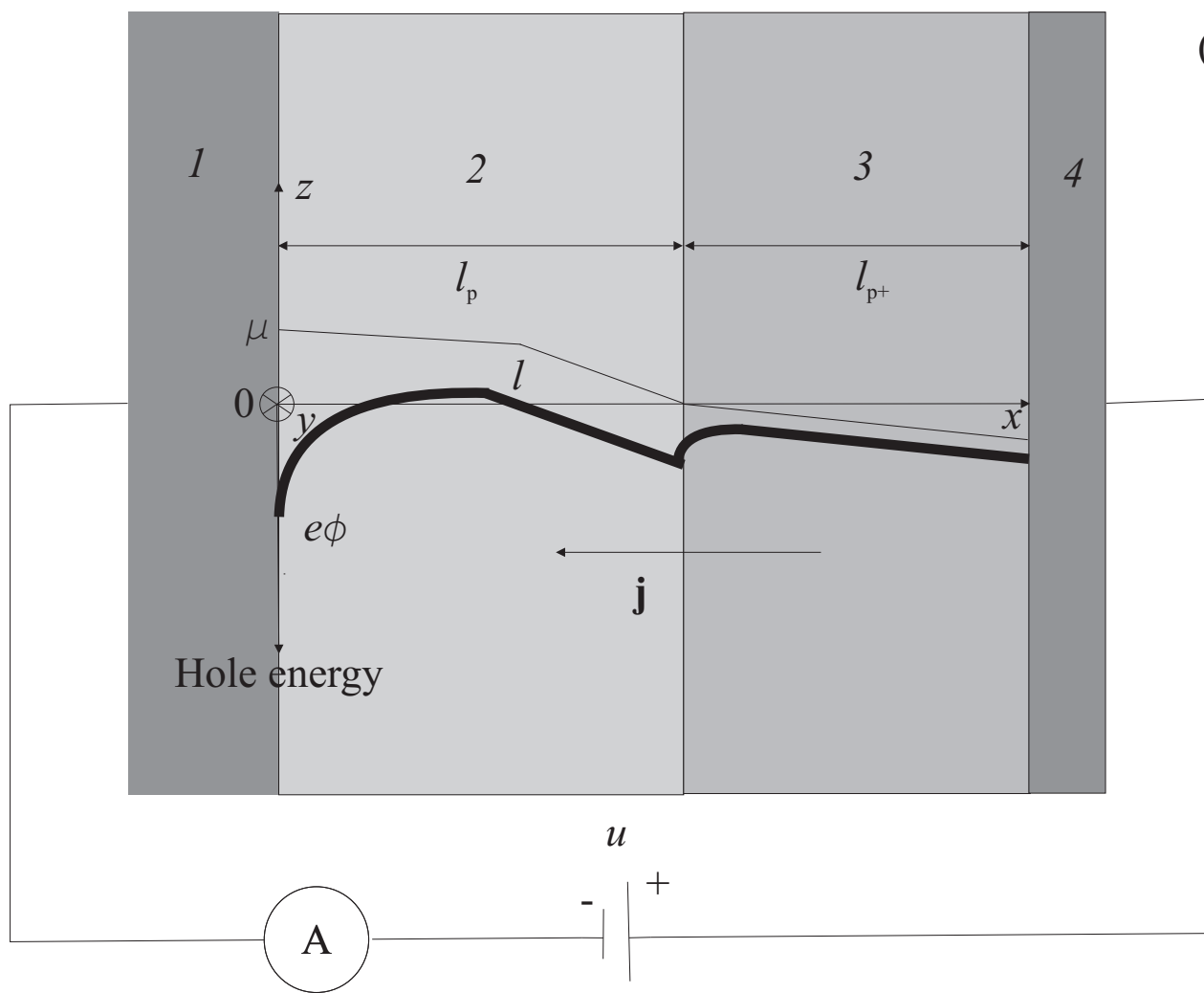
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