

Applied Mathematics and Nonlinear Sciences

<https://www.sciendo.com>

Electronic properties of diamond semiconductor materials: based on response surface model

Sheng Bi¹, Xiaoying Ye¹, Yang Shao^{1,†}

1. Tangshan Polytechnic College, Tangshan 063299, China

Submission Info

Communicated by Z. Sabir

Received March 11, 2022

Accepted July 17, 2022

Available online March 20, 2023

Abstract

Diamond, a wide bandgap semiconductor material, has excellent physicochemical properties. It has great potential for application in high temperature, high frequency, high power electronic devices and other high technology fields. In order to study the electronic properties of diamond more precisely, an AM-response surface model is developed in this paper to investigate the electronic structures of diamond, P-doped diamond and N-doped diamond surfaces in depth. It is shown that there are three forms of charge states in the single vacancy on the diamond surface. When $E=0$ V, the negative charge energy level is -0.5 mV, the positive charge is 1 mV, and the zero level remains 0 . And its energy level is unstable. In contrast, the double vacancy charge on the diamond surface varies depending on the valence band taken by E , and only one charge state exists. When $E<0$, the diamond surface vacant electron nature is negative charge state. When $E>0$, it is positive charge energy level. The electronic properties of the P-doped diamond semiconductor material are calculated to have a constant positive charge (1 mV). The electronic property of N-doped diamond semiconductor material is constant negative charge (-1 mV).

Keywords: diamond; semiconductor materials; AM algorithm; response surface model; electronic properties

AMS 2020 codes: 81S30

[†]Corresponding author.

Email address: 15100526039@139.com

1 Introduction

Semiconductor materials possess excellent electrical and optical characteristics because of their stable structure and rich physical connotation [1-2]. And their low prices enable them to have broad applications in new energy, optical devices, integrated circuits, etc. in production life. It is a meritorious material that drives human society into a new era of a new production and lifestyle [3-4]. The first generation of silicon-based semiconductors was with diamond-type structure and they were successfully applied to make integrated circuits, which brought a great contribution to the development of computer industry and network engineering [5-6]. However, because they are inherently indirect bandgap semiconductors limit their luminescence efficiency in the photoelectric conversion process, and silicon transmission is slow and single-function [7-8]. The second generation semiconductor materials are represented by gallium arsenide, which are materials with direct band gap of sphalerite structure and can be used in light-emitting devices. The third-generation semiconductor materials represented by gallium nitride are new semiconductor materials developed after silicon-based and gallium arsenide semiconductors [9-10]. They can be prepared into two structures at atmospheric pressure, which are fibrillated zincite type and sphalerite type. However, the strength and toughness of the above semiconductor materials have disadvantages. While diamond has very high hardness and refractive index, it has a wide range of applications in jewelry, industry, and scientific instruments [11-12]. And it has played a revolutionary role in promoting the industries such as drilling and mining, machining and electronic devices. It has been shown that diamond, as a new semiconductor material, has a wide range of application prospects due to its excellent properties [13-14]. The results of the literature search on “diamond semiconductor materials” in China Knowledge Network are shown in Tab. 1 [15-16]. From Tab. 1, we can see that in 2022, there are 4507 articles related to “diamond semiconductor materials”, so it is clear that the scientific research on “diamond semiconductor materials” is relatively cutting-edge and has far-reaching research value [17-18].

Table 1. Number of literatures on the topic of “diamond semiconductor materials”, 2018-2022

year	Number (thousands of articles)
2018	0.342
2019	0.678
2020	1.327
2021	3.012
2022	4.507

Diamond is a semiconductor material with excellent properties such as wide band gap, high thermal conductivity, high carrier mobility, room temperature hole mobility (5 times higher than silicon) and unique surface conductivity [19-20]. The operating temperature can reach 300-400°C (the highest silicon device is only 200°C), and the quality factor of microwave power devices is 700 times higher than that of arsenide graft and 800 times higher than that of silicon, and so on. With the rapid development of modern science and technology, the requirements for high temperature resistance, radiation resistance, ultra-high speed and high-power semiconductor devices and integrated circuits with high integration have been increasing [21-22]. Both scientific and industrial communities have recognized that diamond wide bandgap semiconductor materials and devices are the most promising semiconductor materials with very attractive development prospects. However, natural diamonds usually require hundreds of millions or billions of years of crystallization under extremely high pressure and temperature in the Earth’s lithosphere and are carried to the surface by lava from volcanic eruptions [23-24]. Moreover, the purity and homogeneity of natural diamonds are difficult to reach the optical magnitude, thus limiting their applications in many fields including optical

windows, lenses, and sensing. In the past decade or so, the growth technology of single-crystal diamond has gradually matured, and now high-quality optical-grade artificial diamond crystals with lengths of more than 1 cm have been obtained [25-26]. Their purity is several orders of magnitude higher than that of the diamonds present in nature. At the same time, the emergence of artificial single-crystal diamond has become an important turning point for people to explore again the application of diamond in the field of semiconductors. According to Pan [27], diamond has a wide range of applications in production life, both as a two-dimensional layered material and as a semiconductor material. Zhang [28] showed that the electronic properties in this diamond are worthy of further investigation by scientists, and the physical mechanism behind these electronic properties is also a new challenge for condensed matter physics. Ohmagari [29] showed that the change in the current signal before and after the reaction on the diamond surface can be measured by electrochemical means. Because of its long-term stability, this system can even be used in sensor systems to track and monitor the dynamics of pathogens in living organisms in real time. This is a breakthrough in the field of molecular biology and biosensor fabrication. It has stimulated the interest in the research of diamond semiconductor materials. According to Lukosi [30], diamond is the most promising semiconductor material in recent years as a wide-bandgap semiconductor with a wide range of applications for military fields as well as for production life. Therefore, the investigation of the electronic properties of such semiconductor materials has profound implications for the understanding of such materials and their applications.

In the previous semiconductor electronic property tests, a lot of human and material resources are required to figure out the experimental conditions, which results in higher experimental costs. If the phase transition test points can be predicted theoretically, the consumption of materials as well as costs can be directly reduced [31-32]. The response surface model can perfectly solve the above problems. Response surface models are mainly used to establish the mapping relationship between the structure and charge of semiconductor materials [33-34]. And an experimental technical tool based on statistical analysis is established. The computational process of the response surface model is: first, sufficient sample points of design parameters are selected within the range of semiconductor parameters taken in the finite element model. Selection of specific structural response values as sample electronic property parameters. Then, the semiconductor parameter sample points are brought into the response surface model to calculate the corresponding structural response values to form the structural response sample space [35]. The explicit functional relationship between the semiconductor parameter samples to the structural response samples, i.e., the response surface model, is established by the function fitting tool, which can be used as a proxy model for the electronic property parameters of semiconductor materials.

Based on the above research background, this paper establishes the AM-response surface model based on the conduction function in the capture theory and conducts an in-depth study on the electronic properties of diamond semiconductor materials. The study mainly covers the electronic structure of diamond, P-doped diamond and N-doped diamond surfaces. And specifically analyze the effect of different vacancies and doping ions on their electronic properties.

2 Response surface model study based on the derivative function

The most fundamental physical processes in diamond semiconductors are charge carrier injection and transport, and they have a very direct and critical impact on the performance characteristics of the material such as brightness, efficiency, energy dissipation, and lifetime. Since, the thin film structure of diamond semiconductors is disordered and amorphous, the physical processes of charge carrier transport become more complicated compared to the conventional inorganic semiconductor materials. Therefore, in this paper, a response surface model is developed based on the conduction function in

the capture theory. A computational study of the electronic properties of diamond semiconductor materials is carried out.

2.1 Capture theory study

The capture currents are classified into two categories, injection-limited and bulk-limited, according to the reasons for current limitation in semiconductor materials. When the charge carrier mobility of the material is high and there is no space charge inside the device to form the opposite electric field, the device current is mainly determined by the injection at the interface. Generally, the interface potential barrier is higher at this time, which is called injection-limited current. Conversely, when the interface potential barrier is low, i.e., the quasi-ohmic contact state, it is easy for charge carriers to be injected from the interface at this time. However, because of its more difficult transmission inside the device, the opposite electric field space charge is quickly formed, preventing further injection and transmission of charge carriers from the interface. This current is called the body-limited current. This is the basic space charge limiting current. In addition, the purity of the diamond semiconductor material is not very high, impurities exist, as well as the material tends to crystallize during the coating process. Therefore, there are a large number of defects in the general film, which causes the transport process of charge carriers in organic thin film devices to appear more cumbersome. For this reason, a transport model based on diamond semiconductors is proposed. Among them, the trap capture theory describing the current-voltage characteristics of organic semiconductor devices is the most common.

The trapping theory is mainly based on Poisson's equation and current density equation, which describe the transport process of organic semiconductor charge carriers under traps with inhomogeneous spatial distribution. Poisson's equation and current density equation for the single-carrier, trapped case is given below.

$$\frac{\varepsilon}{q} \cdot \frac{\partial E(x)}{\partial x} = \rho(x) + \rho_t(x) \quad (1)$$

$$J = q\mu\rho(x)E(x) \quad (2)$$

Where $E(x)$ is the electric field strength, J is the current density, V is the DC bias voltage, $\rho(x)$ is the charge carrier density, $\rho_t(x)$ is the captured carrier density, μ is the carrier mobility, d is the sample thickness, ε is the dielectric constant of the sample, and q is the meta-charge. The boundary conditions are shown below.

$$V = \int_0^a E(x)dx \quad (3)$$

(a) If the presence of the trap is not considered (ideal case), $\rho_t(x)=0$, Poisson's equation can be written as.

$$\frac{\varepsilon}{q} = \frac{\partial E(x)}{\partial x} = \rho(x) \quad (4)$$

At this point, solving equations (2), (3) and (4) yields.

$$J = \frac{9}{8} \varepsilon u \frac{V^2}{d^3} \quad (5)$$

Eq. (5) is the Mott-Gurney equation, also known as the square law for the space-charge-limited current in the absence of traps.

(b) Traps confined to single and multiple discrete energy levels

In this case, the trap is considered to be discrete in energy and uniform in space, then the current-voltage characteristic can be expressed as.

$$J = \frac{9}{8} \varepsilon \mu \frac{V^2}{d^3} \theta \quad (6)$$

Where $\theta = \frac{\rho(x)}{\rho_t(x) + \rho(x)}$. If the traps are spatially inhomogeneously distributed, the sample thickness should be converted to the effective thickness.

(c) Traps with exponential distribution in the forbidden band energy gap

The current-voltage characteristics in this case are expressed as.

$$J = q^{1-l} \mu N_v \left(\frac{2l+1}{l+1} \right)^{l+1} \left(\frac{l}{l+1} \frac{\varepsilon}{H_b} \right)^l \frac{V^{l+1}}{d^{2l+1}} \quad (7)$$

Where $l = T_c/T$, T_c are the characteristic constants of the distribution and H_b is the trap density.

(d) Trap with Gaussian distribution in the forbidden band energy gap

In case of shallow traps, the current-voltage characteristics in this case are expressed as.

$$J = \frac{9}{8} \varepsilon \mu \frac{V^2}{d^3} \theta \quad (8)$$

In case of a deep trap, the current-voltage characteristic in this case is expressed as.

$$J = q^{1-m} \mu N_v \left(\frac{2m+1}{m+1} \right)^{m+1} \left(\frac{m}{m+1} \frac{\varepsilon}{H_b} \right)^m \frac{V^{m+1}}{d^{2m+1}} \quad (9)$$

Where $m = (1 + 2\pi\sigma_t^2/16k^2T^2)^{1/2}$.

2.2 Conductivity function study

The admittance function (AM) is one of the capture algorithms with a small amplitude sine wave as the detection signal. The system to be investigated is studied by establishing the relationship function between the detection signal and the output signal to obtain the conductance (impedance) information

over a wide frequency range. It is also important to note that the AC probe signal applied to the system to be studied is so small that its effect on the system can be basically ignored.

This paper is mainly based on the conductance function to study diamond semiconductor materials. A small amplitude AC voltage signal $v(t) = V_m \sin(\omega t)$ is applied to the organic semiconductor sample to be measured, and a small amplitude AC current signal $i(t) = I_m \sin(\omega t + \theta)$ will be generated at the same time, and the phase difference between the two signals is θ . The conductance is defined as the ratio of the output current signal to the input voltage signal, i.e., $Y(\omega) = \frac{i_{ac}}{v_{ac}} = G + iB$, where G is the conductance, B is the conductance, and ω is the angular frequency. There is a relationship between the conductance and capacitance and the angular frequency $B = \omega C$, C is the capacitance. In this way, it is obvious from the equations that the conductance is closely related to the conductance and capacitance, and many electrical properties of organic semiconductors are related to the conductance and capacitance, thus the conductance wave spectroscopy establishes the connection between the electrical parameters within organic semiconductors, which is extremely important for the study.

Experimental direct measurements of the conductance information spectra of the studied systems are generally available in only one form. A variety of different spectral curves can be transformed according to the relationship of the conductance-nano function (10), which makes it possible to study and analyze the experimental data more effectively and to better reflect the electrical properties of the system in many ways.

$$\frac{1}{Z} = Y(\omega) = \frac{i_{ac}}{v_{ac}} = G + iB = G + i\omega C \quad (10)$$

Specific conductance spectral curves are often used in the following forms: conductance-frequency curve $(G - f)$, capacitance-frequency curve $(C - f)$, normalized capacitance-frequency curve $(C/C_{geo} - f)$, negative differential conductance-frequency curve $(-\Delta B - f)$, conductance/frequency-frequency curve $(G/f - f)$, and so on. From the different forms of conductance spectra, we can well analyze the characteristics of the studied system, such as negative capacitance phenomenon, interfacial activation energy magnitude, carrier mobility, and so on.

Based on the theory of space charge-limited currents, the conductance model (13) is obtained based on the current density equation (11) and Poisson's equation (12), and then by Fourier transform.

$$J(t) = q\rho(x,t)\mu(t)E(x,t) + \varepsilon \frac{\partial E(x,t)}{\partial t} \quad (11)$$

$$\rho(x,t) = (\varepsilon / q) \frac{\partial E(x,t)}{\partial x} \quad (12)$$

Where $\Omega = \omega\tau_t$ is the normalized frequency, $\tilde{\mu}(\Omega)$ is the normalized carrier mobility, and M and α are the dispersion parameters of the material, where $M = 0$, $\alpha = 1$, and τ_t are the steady-state carrier migration times for trap-free non-dispersive transport.

$$Y(\Omega) = \frac{\varepsilon A}{\tau_t d} \left(\frac{\Omega^3}{2i[\tilde{\mu}(\Omega)]^2 \{1 - \exp[-i\Omega / \tilde{\mu}(\Omega)]\} + 2\tilde{\mu}(\Omega)\Omega - i\Omega^2} \right) \quad (13)$$

Where,

$$\tilde{\mu}(\Omega) = \frac{\mu(\Omega)}{\mu_{dc}} = 1 + M (i\omega\tau_t)^{1-\alpha} \quad (14)$$

2.3 Response surface model study based on the conductivity function

Ideally, the organic layer is trap-free. However, because the purity of organic semiconductor materials is not particularly high, and because of the defects that may arise during the preparation of organic thin films, the influence of traps cannot be ignored when establishing the theoretical admittance (AM)-response surface model. Assuming the exponential distribution of traps and considering the electric field-dependent characteristics of carrier mobility, the conductance model with single carrier transport and exponential trap distribution is established. At this point, the current density equation and Poisson's equation take the following form.

$$J(t) = q\rho(x,t)\mu E(x,t) + \varepsilon \frac{\partial E(x,t)}{\partial t} \quad (15)$$

$$(\varepsilon / q) \frac{\partial E(x,t)}{\partial x} = \rho(x,t) + \rho_t(x,t) \quad (16)$$

The trap state dynamics process is described by the following equation.

$$d\rho_t / dt = c_p (N_t - \rho_t) - e_p \rho_t \quad (17)$$

The AM-response surface model is built under these three assumptions: (1) no trap, (2) single carrier injection, and (3) carrier mobility versus concentration $\mu = an^b$. Similarly, the steady-state current density equation, derived from Poisson's equation and the current density equation through complex mathematical and theoretical equations, is obtained as follows.

$$J = a\varepsilon \left(\frac{\varepsilon}{q} \right)^b \frac{(b+1)^{b+1} (2b+3)^{b+2} V^{b+2}}{(b+2)^{2b+3} L^{2b+3}} \quad (18)$$

When b takes 0, (18) becomes the well-known Mott-Gurney equation.

After adding the small AC voltage signal, the theoretical conductance model obtained by the tedious derivation of the equations is.

$$Y(\Omega) = \text{Re} \left(\frac{1}{(2b+3)v(\Omega)} \right) A \frac{dj_{ac}}{dV} + i\omega \text{Im} \left(\frac{1}{\Omega v(\Omega)} \right) C_{geo} \quad (19)$$

Previously established theoretical conductance models have ignored the influence of the interface on the charge carriers, considering that the interface is in ohmic contact; in fact, the state of the interface has a very important influence on the charge transport. Based on the single carrier injection conduction model, the influence of the interface state needs to be considered. The AM-response surface model is established. The interface state properties are shown as follows.

$$g(E_2^r - E_2) = \frac{N_1}{k_B T_0} \exp\left[-(E_2^r - E_2)/k_B T_0\right] \quad (20)$$

Similarly, after a complex derivation of the equations, the following AM-response surface model is obtained.

$$Y = q \int_{-\infty}^{+\infty} g_1(E_2^r - E_2) \left(\frac{\partial v_{12}}{\partial \theta}(E_2) \frac{\Delta \theta}{\Delta V}(E_2) + \frac{\partial v_{12}}{\partial V}(E_2) \right) dE_2 \quad (21)$$

The AM-response surface model is a powerful electrical measurement tool, and the conductance information enables to obtain many electrical parameters about organic semiconductor materials, such as capacitance, conductance, electronegativity, impedance, etc. Based on this information, there are many applications in organic semiconductor research, as follows.

According to the above equation, the single carrier AM-response surface model at trapless is obtained as follows.

$$Y(\Omega) = \frac{\varepsilon A}{\tau_{dc} d} \left(\frac{\Omega^3}{2i[0.75\tilde{\mu}(\Omega)]^2 \{1 - \exp[-i4\Omega/3\tilde{\mu}(\Omega)]\} + 1.5\tilde{\mu}(\Omega)\Omega - i\Omega^2} \right) \quad (22)$$

Where $\tilde{\mu}(\Omega) = \frac{\mu(\Omega)}{\mu_{dc}} = 1 + M(i\omega\tau_{dc})^{1-\alpha}$ and $\Omega = \omega\tau_{dc}$ are the normalized frequencies, M and α are the dispersion parameters of the material, and τ_{dc} is the steady-state carrier migration time.

Space-charge-limited current theory based on single-carrier transport. The impedance of organic semiconductor thin film devices with only single carrier transport can be described by the following equation.

$$Z = 6\psi R_i \sum_{k=0}^{\infty} \frac{1}{k+3} \frac{\Gamma(\psi+1)}{\Gamma(\psi+k+2)} \left(\frac{\psi}{\delta}\right)^k (-i\Omega)^k \quad (23)$$

Where Γ is the Eulergamma function, R_i is the resistance increment in the low frequency region, ψ and δ are the capture parameters, $\Omega = \omega\tau$.

At low frequencies ($2\pi f \ll 1$), the first term of the above equation dominates, so there is an impedance $Z = 2R_i\psi / (1+\psi)$, and because $Y = 1/Z = G + i\omega C$, there is

$$G(\omega) = \frac{1}{2R_i\delta} \left[\frac{1+A}{(1+A)^2 + B^2} + \delta \right] \quad (24)$$

$$C(\omega) = \frac{1}{2R_i\delta\omega} \frac{B}{(1+A)^2 + B^2} \quad (25)$$

In the above equation, $A = \int_{E_v}^{E_c} N_t(E) S_t v_{th} \gamma_t(E) / [\gamma_t(E)^2 + \omega^2] dE$,

$B = \omega \int_{E_v}^{E_c} N_t(E) S_t v_{th} / [\gamma_t(E)^2 + \omega^2] dE$, E_c is the conduction band energy levels, E_v is the valence band energy level, S_t is the capture cross section area, v_{th} is the electron thermal motion velocity, and γ_t is the release probability.

$$\frac{\partial \omega B}{\partial \omega} = N_t(E_0) S_t v_{th} \frac{kT}{\omega} \quad (26)$$

From equations (24), (25) and (26), the constant domain state distribution is obtained as.

$$N(E_0) = \frac{2R_i \omega}{S_i v_{th} \delta kT} \frac{\partial}{\partial \omega} \left\{ \frac{\omega^2 C(\omega)}{[2R_i \omega C(\omega)]^2 + [2R_i G(\omega) - 1]^2} \right\} \quad (27)$$

In addition,

$$E_c - E_0 = kT \ln(v / \omega) \quad (28)$$

Substituting the conductance $G(\omega)$ and capacitance $C(\omega)$ into (27) and (28), the fixed domain state distribution, the impedance information of the device and the fixed domain state part are obtained.

For modeling purposes, the AM-response surface model for anode ohmic contact single carrier injection (in the case of cavities) without traps will be derived in detail. A one-dimensional model is used, with the plane located at $x = 0$ as the cavity injection interface (anode). The plane located at $x = L$ is used as the collecting interface (anode), and the sample thickness is L . Since the anode is an ohmic contact, $E(x = 0, t) = 0$.

Electric field dependent mobility.

$$\mu(E) = \mu_0 \exp(\gamma \sqrt{E}) \quad (29)$$

$$\mu(E_{dc} + \hat{E}) = \mu(E_{dc}) + \frac{\partial \mu}{\partial E_{dc}} \hat{E} \quad (30)$$

$$\frac{\partial \mu}{\partial E} = \frac{\gamma}{2} \mu(E) \frac{1}{\sqrt{E}} \quad (31)$$

In this way, the AM-response surface model (30) equation can be described as $Y = Y(\varepsilon, L, S, f, \tau)$, where only one migration time is a variable and all others are known quantities. However, dispersive transport not only produces a widely distributed migration time, but also gives rise to a time- (frequency)-dependent mobility $\mu(\omega)$. Considering again that the mobility is related to the electric field, the mobility can be written in the form of $\mu(\omega, E)$. Separating time and electric field gives $\mu(\omega)\mu(E)$, where $\tilde{\mu}(\omega) = 1 + M(i\omega\tau)^{1-\alpha}$.

In this way, under DC conditions, $\tilde{\mu}(\omega) = 1$.

Solving (29), (30), (31) yields.

$$J = \frac{9}{8} \varepsilon \mu(E_{dc}) \frac{V^2}{d^3} \quad (32)$$

$$E_{dc}(x) = \sqrt{\frac{2J}{\varepsilon \mu(E_{dc})}} x^{1/2} = \frac{3V}{2L^{3/2}} x^{1/2} = \frac{3\sqrt{L}}{2\tau \mu(E_{dc})} x^{1/2} \quad (33)$$

Based on a large number of algorithmic studies, this section introduces the basic concepts and fundamentals of the conductivity function in detail. It also summarizes the specific applications of the AM-response surface model in the study of diamond semiconductors. The measurement of carrier mobility of diamond semiconductors and the study of fixed domain state distribution of organic semiconductors are presented. Finally, a detailed derivation of the process of building a single-carrier AM-response surface model without traps and an analytical discussion of it are presented. This section provides a general and systematic introduction to the conductivity function and how to use the AM-response surface model to study diamond semiconductors.

3 Diamond semiconductor material electronic properties research

3.1 Study of electronic properties of diamond surface vacancies

As the dimensionality of microelectronic devices continues to decrease and the specific surface area increases. The effect of diamond surface defects on their electronic properties becomes more and more prominent. Vacancy is an important defect. Its effect on the growth and electronic properties of diamond semiconductor materials is obvious. Therefore, it is of far-reaching significance to study the electronic properties of diamond surface vacancies from a microscopic perspective. In this paper, the AM-response surface model is developed based on the capture theory using a double-precision AM function. AM function is expanded according to an exact numerical basis set. For the numerical integration we use a medium precision grid. A $2 \times 2 \times 3$ grid generated by the Mott-Gurney equation was used for both structural optimization and single electric energy calculations. Parallel hexahedral method was used for electron density calculations. Only a 3-layer grid was applied for calculating the electron properties.

The calculated electronic properties of diamond at single vacancy are shown in Figure 1. The calculation of the single vacancy charge on the diamond surface by the AM-response surface model reveals that it can exist in the form of three charge states: i.e., positive, zero and negative charge. This indicates that the electronic properties of the diamond surface vacancy can be carried out by the change of the charge state. From Figure 1, when $E = 0$ V, the negative charge energy level is -0.5 mV, the positive charge is 1 mV, and the zero position remains 0. This indicates that the nature of the vacancy electrons on the diamond surface depends on the charge state and the magnitude of the Fermi energy level E . When E is certain, the lower the charge state is, the lower the formation energy is. As E gradually increases, the formation energy of the positive charge state increases. This indicates that the negative charge state formation energy decreases. It means that it is more difficult to exist stable electronic properties. Therefore, it can be concluded that multiple charge states can exist in diamond surface vacancies. Regardless of the value of the Fermi energy level E , the electronic nature of the single vacancy on the diamond surface is unstable.

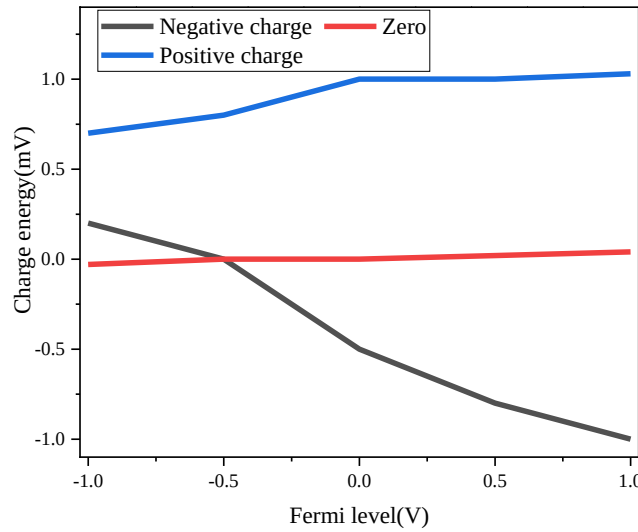


Figure 1. Analysis of electronic properties at single vacancies on the surface of diamond

By removing two atoms from the linked structure of diamond semiconductor material, a double vacancy structure is formed. The calculated electronic properties at double vacancies on the diamond surface are shown in Figure 2. The calculation of the diamond surface double vacancy charge by the AM-response surface model reveals that it can exist in three charge state forms: i.e., positive charge, zero-site and negative charge. However, unlike Figure 1, only one charge state exists in the diamond surface vacancy according to the valence band value taken for E . That is, when $E < 0$, the negative charge energy level is -1 mV, the positive charge is 0 mV, and the zero position is 0. That is, when $E < 0$, the negative charge energy level is -1 mV, the positive charge is 0 mV, and the zero position is 0. The electronic nature of the diamond surface vacancy is a negative charge state. When $E > 0$, the negative charge energy level is 0 mV, the positive charge is 1 mV, and the zero position is 0. The electron nature of the diamond surface vacancy is a positive charge state. In addition, the total energy of double vacancies is higher than that of single vacancies. It means that they are the most stable form of electrons.

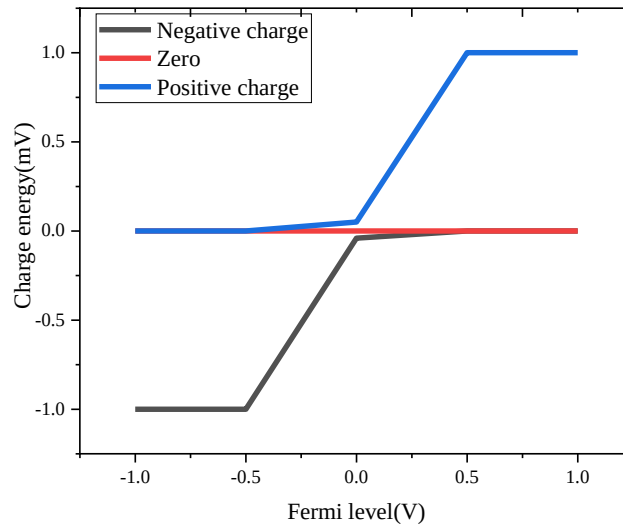


Figure 2. Analysis of electronic properties at double vacancies on diamond surface

3.2 Study of electronic properties of ion-doped diamond

From the calculation, it is clear that defects exist on the surface of undoped diamond semiconductor materials. They can be classified as single vacancy defects and double control defects. In order to make the diamond semiconductor material more stable, the ions are doped in the diamond semiconductor and used to fill the defective vacancies. This measure has attracted the attention of researchers. Therefore, in this section, the electronic properties of ion-doped diamond are calculated by AM-response surface model. The commonly used doping ions are P-ion, N-ion, and Na-ion. Since Na-doped diamond, which requires high activation energy, is not suitable for use at room temperature. Therefore, in this paper, P ions and N ions are selected to be brought into the AM-response surface model for calculation. The calculation results are shown in Figure 3 and Figure 4. Figure 3 shows the calculation results of electronic properties of P-doped diamond semiconductor material. From Figure 3, it can be seen that the P-doped diamond semiconductor material has only one state of charge, i.e., positive charge state. When $E > 0$, the positive charge energy level is constant at 1 mV, and the energy level of the negative charge and zero position is constant at 0 regardless of the value of E . This indicates that the P-doped diamond semiconductor material allows all atoms to move freely until the system energy reaches its maximum during the structure optimization process.

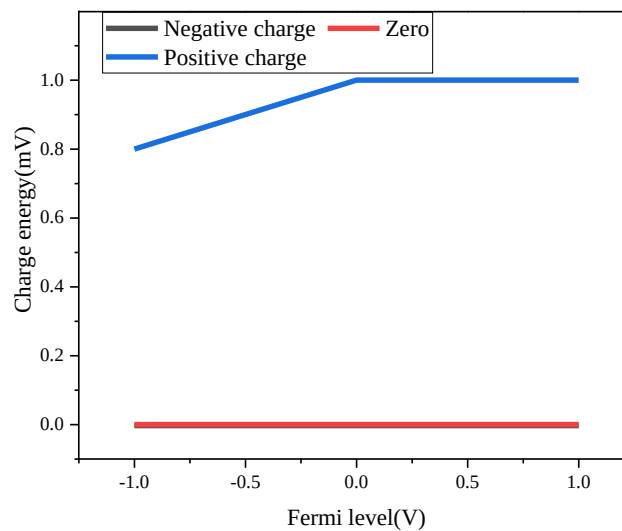


Figure 3. Analysis of electronic properties of P-doped diamond

Figure 4 shows the calculated electronic properties of N-doped diamond semiconductor materials. From Figure 4, it can be seen that the charges of N-doped diamond semiconductor materials are all negative charge energy levels. This indicates that the structure of the material allows all atoms to move freely during the growth of the P-doped diamond material until the energy of the system reaches the minimum.

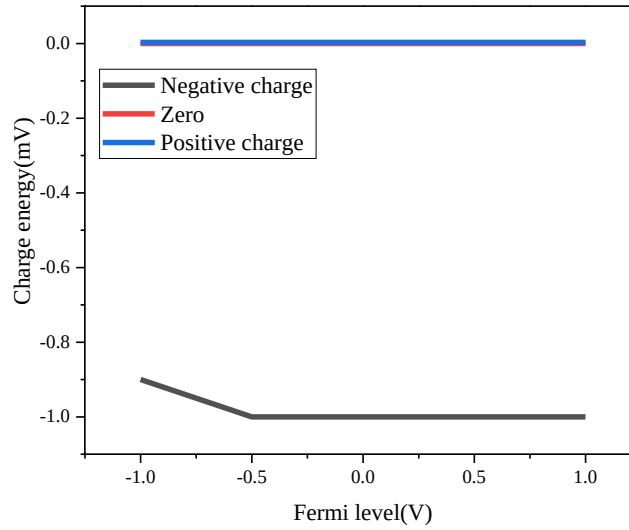


Figure 4. Analysis of electronic properties of N-doped diamond

4 Conclusion

In this paper, an AM-response surface model is developed based on the conductance (AM) function of the capture theory. The electronic structures of diamond, P-doped diamond and N-doped diamond surfaces were calculated. The effects of different vacancies and doping ions on their electronic properties were specifically analyzed. Specific conclusions are as follows.

- 1) Calculation of the single vacancy charge on the diamond surface by the AM-response surface model reveals that it can exist in three charge state forms: i.e., positive, zero, and negative charge. When $E=0$ V, the negative charge energy level is -0.5 mV, the positive charge is 1 mV, and the zero position remains 0. This suggests that the nature of vacant electrons on the diamond surface depends on the charge state and the magnitude of the Fermi energy level E . Therefore, the electronic properties of the single vacancies on the diamond surface are unstable regardless of the value of the Fermi energy level E .
- 2) The model calculates the double vacancy charge on the diamond surface and finds that only one charge state exists in the vacancy on the diamond surface according to the valence band value of E taken. When $E < 0$, the negative charge energy level is -1 mV, the positive charge is 0 mV, and the zero position is 0. The nature of the vacant electrons on the diamond surface is a negative charge state. When $E > 0$, the negative charge energy level is 0 mV, the positive charge is 1 mV, and the zero position is 0.
- 3) The calculation shows that the P-doped diamond semiconductor material has only one state of charge, i.e., the positive charge state. When $E > 0$, the positive charge energy level is constant at 1 mV. The charges of N-doped diamond semiconductor materials are all negative charge energy levels. When $E < 0$, the energy level of negative charge is constant at -1 mV, and the energy level of positive charge and zero position is constant at 0 regardless of the value of E . This indicates that during the growth of P-doped diamond semiconductor materials, the material structure allows all atoms to move freely until the energy of the system is minimized.

References

- [1] Qian, T., et al. (2022). Resilient decentralized optimization of chance constrained electricity-gas systems over lossy communication networks. *Energy*, 239, 122158.
- [2] Qian, T., et al. (2019). Event-triggered updating method in centralized and distributed secondary controls for islanded microgrid restoration. *IEEE Transactions on Smart Grid*, 11.2, 1387-1395.
- [3] Fang, Ch., et al. (2021). Mapping Relation of Leakage Currents of Polluted Insulators and Discharge Arc Area. *Frontiers in Energy Research*, 9, 777230.
- [4] Zhou, W. (2020). *Chinese Independent Animation: Renegotiating Identity in Modern China*. Springer Nature.
- [5] Cheng, J., et al. (2020). Optical, electronic properties and anisotropy in mechanical properties of “X” type carbon allotropes. *Materials*, 13.9, 2079.
- [6] Kundu, A., et al. (2022). Influence of nuclear quantum effects on the electronic properties of amorphous carbon. *Proceedings of the National Academy of Sciences*, 119.31, e2203083119.
- [7] Qiu, D., et al. (2018). Structural and electronic properties of two-dimensional (110) diamond nanofilms by first-principles calculations. *Diamond and Related Materials*, 84, 55-61.
- [8] Li, J., et al. (2022). First principles on the structure and electronic properties of vertically regulated two-dimensional cubic boron nitride and diamond like carbon sandwich heterostructures. *Surface Science*, 122146.
- [9] Zhang, M., et al. (2021). Electrical properties of yttrium gate hydrogen-terminated diamond field effect transistor with Al₂O₃ dielectric layer. *Applied Physics Letters*, 118.5, 053506.
- [10] Cui, Z., et al. (2021). Tuning the electronic properties of MoSi₂N₄ by molecular doping: a first principles investigation. *Physica E: Low-dimensional Systems and Nanostructures*, 134, 114873.
- [11] Chen, S., et al. (2019). Progress to electrical properties of diamond-SiC composites under high pressure and high temperature. *Diamond and Related Materials*, 94, 203-208.
- [12] Fan, Q., et al. (2021). Stability, mechanical, anisotropic and electronic properties of oP8 carbon: A superhard carbon allotrope in orthorhombic phase. *Journal of Solid State Chemistry*, 294, 121894.
- [13] Chiesa, M., et al. (2020). Nitrogen-doped semiconducting oxides. Implications on photochemical, photocatalytic and electronic properties derived from EPR spectroscopy. *Chemical Science*, 11.26, 6623-6641.
- [14] Zkria, A., et al. (2020). Analysis of electrical characteristics of Pd/n-nanocarbon/p-Si heterojunction diodes: By CVf and G/wVf. *Journal of Nanomaterials*.
- [15] Lyons, J. L. (2019). Electronic properties of Ga₂O₃ polymorphs. *ECS Journal of Solid State Science and Technology*, 8.7, Q3226.
- [16] Ren, Z., et al. (2020). High temperature (300° C) ALD grown Al₂O₃ on hydrogen terminated diamond: Band offset and electrical properties of the MOSFETs. *Applied Physics Letters*, 116.1, 013503.
- [17] Sun, Z., et al. (2022). Electrical Characteristics of Metal Contacts to Carbon Nanowalls. *ECS Journal of Solid State Science and Technology*, 11.6, 061012.
- [18] Ghorbani, M., et al. (2018). 12 Methods of Measuring Electrical Properties of Material. *Electrical Conductivity in Polymer-Based Composites: Experiments, Modelling, and Applications*, 365.
- [19] Guerra, T., et al. (2019). Magnetic and electronic properties of diamond-shaped graphene-boron nitride nanoribbons and nanoflakes. *Journal of Physics and Chemistry of Solids*, 135, 109085.
- [20] Pierucci, D., et al. (2018). Van der Waals epitaxy of two-dimensional single-layer h-BN on graphite by molecular beam epitaxy: Electronic properties and band structure. *Applied Physics Letters*, 112.25, 253102.
- [21] de Vasconcelos, F. M., et al. (2019). Electronic properties of tetragraphene nanoribbons. *Physical Review Materials*, 3.6, 066002.
- [22] Yang, Y., et al. (2021). First-principles study on the electronic properties and enhanced ferromagnetism of alkali metals adsorbed monolayer CrI₃. *Vacuum*, 194, 110561.
- [23] Sharma, V., et al. (2019). Chemical ordering and electronic properties of lone pair chalcogenide semiconductors. *Progress in Solid State Chemistry*, 54, 31-44.
- [24] Ashcheulov, P., et al. (2020). Low temperature synthesis of transparent conductive boron doped diamond films for optoelectronic applications: Role of hydrogen on the electrical properties. *Applied Materials Today*, 19, 100633.

- [25] Qiao, F., et al. (2019). Tunability in the optical and electronic properties of ZnSe microspheres via Ag and Mn doping. *ACS omega*, 4.7, 12271-12277.
- [26] Bafekry, A., et al. (2020). Investigation of strain and doping on the electronic properties of single layers of C 6 N 6 and C 6 N 8: a first principles study. *RSC advances*, 10.46, 27743-27751.
- [27] Pan, Y., et al. (2019). The structure, mechanical and electronic properties of WSi₂ from first-principles investigations. *Vacuum*, 167, 374-381.
- [28] Zhang, G., et al. (2022). Mechanical and electronic properties of α -M₂X₃ monolayers. *Physical Review B*, 105.23, 235303.
- [29] Ohmagari, S., et al. (2018). Large reduction of threading dislocations in diamond by hot-filament chemical vapor deposition accompanying W incorporations. *Applied Physics Letters*, 113.3, 032108.
- [30] Lukosi, E., et al. (2019). Methylammonium lead tribromide semiconductors: Ionizing radiation detection and electronic properties. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 927, 401-406.
- [31] Pham, K. D., et al. (2018). Layered graphene/GaS van der Waals heterostructure: controlling the electronic properties and Schottky barrier by vertical strain. *Applied Physics Letters*, 113.17, 171605.
- [32] Botella, P., et al. (2019). High-pressure characterization of the optical and electronic properties of InVO₄, InNbO₄, and InTaO₄. *SN Applied Sciences*, 1.5, 1-12.
- [33] Ameni, B., et al. (2022). A new supramolecular semi conductor cobalt organometallic complex: Structural study, optical and electrical properties. *Journal of Molecular Structure*, 1266, 133518.
- [34] Idrissi, S., et al. (2021). Sulfur doping effect on the electronic properties of zirconium dioxide ZrO₂. *Materials Science and Engineering: B*, 270, 115200.
- [35] Khan, H., et al. (2018). Polypyrrole/MnO₂ composites: synthesis, structural and electrical properties. *Journal of Materials Science: Materials in Electronics*, 29.11, 9090-9098.