PAPER

Analytical modelling of quantum capacitance and carrier concentration in Archimedean zigzag SiC nanoscrolls

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Abstract
Considering the ongoing miniaturization of electronic devices using new categories of nanomaterials, particular importance should be given to the quantum confinement effects in advanced fabrication processes. This paper presents a new analytical model of the quantum capacitance for zigzag silicon doped graphene nanoscrolls, SiCNSs. Although, studying the electronic properties and synthesis methods of SiC-based nanostructures has drawn great research attention in recent years, no analytical model or numerical simulation for quantum capacitance and carrier concentration has been conducted concerning the SiC nanoscrolls so far. In this study, the quantum capacitance model of zigzag SiCNSs is presented for both degenerate and non-degenerate regimes considering the effects of different structural parameters. In the degenerate regime, the zigzag SiCNS shows a constant quantum capacitance value of \(4.75 \times 10^{-11} \text{ F m}^{-1}\) (47.5 pF m\(^{-1}\)) while for non-degenerate regime it follows exponential behaviour. The dominancy of the quantum capacitance of SiCNSs at different levels of concentration is compared in this study. The investigation also highlights the variations of the density of states and carrier concentration with respect to the length and chirality. Presented results suggest that synthesis of SiCNSs possesses a range of potential technological applications as supercapacitors and the channel or interconnections in transistors in the new generation of the nanodevices.

1. Introduction

The rising demand for developed electronics has led the researchers to explore new design approaches using new materials and processes. The current miniaturization of semiconductor electronic devices using these new nanomaterials in advanced fabrication processes greatly improves the overall efficiency and performance of various electronic designs. In this regard, many carbon based materials such as graphene sheets, carbon nanotubes, carbon nanoscrolls and graphene nanoribbons have been used as the channel or interconnections in FETs and MOSFETs in the new generation of the nanoelectronic devices [1–6].

Successful synthesis of graphene and its remarkable physical and electrical characteristics such as large surface area, excellent conductivity, high electron mobility and great mechanical strength has led to increase research interests in discovering new low dimensional materials which share the appealing properties of graphene [7–9]. Carbon nanoscrolls (CNSs) is one such candidate for new generation of nanodevices due to their known specific configuration and special structural, dynamical, and electronic properties [5, 10, 11]. Similar to carbon nanostructured materials, several silicon carbide based nanostructures including nanosprings, nanowires, nanotubes, nanowires and nanobelts have been successfully synthesized using several methods [12–15].

Of the Group IV elements, only carbon can form either sp2 or sp3 bonding and appear in the two-dimensional layered structure. Silicon, the other interesting element of group IV, prefers sp3 hybridization rather than sp2 bonding configuration. Thus, it is not easy to build stable Si structures of nanotubes, nanoscrolls and graphene like sheets. However, it would be practicable to establish layered structures by combining silicon and carbon together [14]. Silicon carbide sheets feature excellent mechanical strength, high electron saturation
velocity, high breakdown electric field and large thermal conductivity. However, it should be considered that nanostructured SiC layers possess even more promising electronic, mechanical and optical properties due to their low dimensionality, shape effect and quantum confinement. Therefore, studying the properties and synthesis methods of SiC-based nanostructures have attracted great research attention these days [16–19].

Recently, many theoretical and experimental studies have been carried out on the electronic properties of SiC nanostructures including the density of state, carrier concentration and conductance mobility [15, 16, 20]. Nevertheless, as far we know, no analytical model or numerical simulation for the mentioned parameters has been conducted concerning the SiC nanoscrolls (SiCNSs) so far. In this study, the density of state (DOS) is derived at first and then it is applied to extract the charge carrier concentration and the quantum capacitance models. The models are presented for both degenerate and non-degenerate regimes considering the effects of different structural parameters.

2. Analytical modeling

CNSs are made by rolling up a single sheet or multiple layers of graphene in the form of Archimedean type spiral. They are topologically open and their core size can be managed through applying external stimuli. In particular, the superior characteristics of nanoscrolls offer a wide range of potential applications such as energy storage and new electronic devices [5, 21–23]. From another point of view, modifying the existing silicon-based technology in the manufacturing process using more efficient nanostructures will help to bring added benefits to the production process of semiconductors. Thus, silicon doped CNSs is predicted to render the new modern technology numerous benefits. Similar to CNSs, it is supposed that the rolling process of a SiCNS is highly involved in two energy contributions, the elastic energy and the free energy that are respectively associated with the layer curvature and the van der Waals interaction. In the initial stage of rolling process, the elastic potential energy increases and consequently the 2D-SiC layer tends to spring back to its original planar shape. Once the edges of the sheet overlap each other, the van der Waals energy predominates the elastic energy and henceforward the overlapping margins firmly adhere to each other. As a result, scrolled SiC structures with high-stability can be formed. Figure 1 represents a common Archimedean scrolled configuration with the general equation of \( r = a + b \theta \) in polar coordinates where \( r \) is the distance from the origin, \( a \) is the start point of the spiral and \( b \) affects the distance between each arm. Regarding the presented equation for Archimedean spiral having \( N \) turns, the distance between each arm is actually given by \( (r - a) / N = 2\pi b \). In general, the exact arc length of a curve \( r(\theta) \) in polar coordinates is specified by:

\[
L = \int_{\theta_{\text{start}}}^{\theta_{\text{end}}} \sqrt{r^2 + \left(\frac{dr}{d\theta}\right)^2} \, d\theta
\]

Where \( \theta \) spans from \( \theta_{\text{start}} \) to \( \theta_{\text{end}} \). Considering the start angle of \( \theta \) as \( \theta_{\text{start}} = 0 \), after \( N \) turns, the end point is \( \theta_{\text{end}} = 2\pi \times N \). Substituting all these together with the derivative in equation (1) gives the total spiral length, \( L \), as:

![Figure 1. Archimedean scrolled configuration of SiC monolayer.](image-url)
Where $a$, as mentioned before, determines the interlayer spacing of the spiral, $b$ is the innermost radius or the starting point of the scroll and $N$ is the number of spiral turns. Moreover, the circumference of the scroll is affected by the chiral vector during the rolling process. Similar to carbon nanostructures [24, 25], a chiral vector can be defined by a chiral index $(n, m)$ using basis vectors $a_1$ and $a_2$ in a silicon carbide sheet. The chiral vector, $\mathbf{C}$, can be denoted as

$$\mathbf{C} = n \hat{a}_1 + m \hat{a}_2$$

where the unit vectors $\hat{a}_1$ and $\hat{a}_2$ are given by:

$$\hat{a}_1 = \left( \frac{3}{2}a_{SiC} \hat{i} + \frac{\sqrt{3}}{2}a_{SiC} \hat{j} \right), \quad \hat{a}_2 = \left( \frac{3}{2}a_{SiC} \hat{i} - \frac{\sqrt{3}}{2}a_{SiC} \hat{j} \right)$$

Where $a_{SiC} = 1.79$ Å is the nearest neighbor Si–C bond length. It should be considered that the structural and electrical properties of each SiCNS can be exclusively determined by the chiral vector and the chiral angle.

Figure 2 characterizes the chirality of the presented silicon carbide nanoscroll. Chiral angle, $\theta$, is defined as the angle between the unit vector of $a_1$ and the chiral vector, $\mathbf{C}$. Regarding the arrangement of edge atoms, there exist three distinct possible categories of Si-doped graphene nanoscrolls, named armchair, zigzag and chiral SiC nanoscrolls. For $m = 0$, nanoscrolls are categorized as zigzag $(n, 0)$ while for those of $n = m$, the SiC nanoscrolls are considered as armchair $(n, n)$. As well, when $n$ is not equal to $m$, SiCNSs fall under the category of chiral $(n, m)$. In terms of chiral angle, $\theta$ is $0^\circ$ and $30^\circ$ for armchair and zigzag nanoscrolls, respectively. Otherwise, if $\theta$ ranges from $0^\circ$ to $30^\circ$, then it is a ‘chiral’ SiCNS.

To start the quantum capacitance modeling, the density of state (DOS) is derived at first for zigzag SiC nanoscrolls. Considering the fact that device scaling brings the dominancy of quantum effect in nano-size device characterization, developing an analytical model for the quantum capacitance and carrier concentration of silicon doped carbon nanoscrolls, SiCNSs, would be of great importance [26–29].

A common expression for quantum capacitance, $C_q$, is presented in equation (4). Accordingly, the quantum capacitance near the charge neutral Dirac point is calculated by taking a differentiation of total carrier concentration relative to the states of energy. Here, $\partial Q = e \partial n_i$ denotes the charge variation, $n_i$ is the carrier concentration and $\partial V = \partial E / e$ represents the applied voltage to the SiCNS while $e$ is the magnitude of the electron charge.

$$C_q = \frac{e^2}{\partial V \partial n_i}$$

To obtain the intrinsic carrier concentration within a band, we start from the parabolic approximation of energy dispersion relation for zigzag SiCNSs. Then, the density of state (DOS) is calculated. Afterward, carrier concentration is derived by integrating the Fermi–Dirac distribution function over all possible energies within a band. The general expression for carrier concentration is given by:
\[ n_i = \int \text{DoS}(E) f(E) \, dE \]  

(5)

Where \( f(E) \) stands as Fermi–Dirac distribution function, also known as Fermi function, providing the probability of an energy level occupation, in thermal equilibrium, by an electron. The Fermi function is defined by 
\[ f(E) = \frac{1}{1 + e^{(E-E_F)/k_BT}}. \]  
Therefore, the structure is characterized by its temperature, \( T \), and its Fermi energy, \( E_F \). The value of Boltzmann’s constant, \( k_B \), is approximately considered as \( 1.3807 \times 10^{-23} \text{ J} \cdot \text{K}^{-1} \).

To develop the energy band structure relation of SiCNSs, \( E(k) \), the two dimensional energy relation of the SiC layer is quantized along the circumference of the scroll. Therefore, initially, it is required to determine the energy band structure of the single layer of SiC. The energy dispersion relation for a silicon-doped graphene sheet using the TB approximation method is calculated as:

\[ E(\vec{k}) = \frac{E_0 + E_0' + \sqrt{(E_0 - E_0')^2 + 12t^2 + 8\pi^2 \cos(\vec{k}(\vec{a}_1 - \vec{a}_2)) - 8\pi^2 \cos(\vec{k} \vec{a}_1) - 8\pi^2 \cos(\vec{k} \vec{a}_2)}}{2} \]  

(6)

Replacing basis vectors of \( \vec{a}_1 \) and \( \vec{a}_2 \) and the wave vector, \( \vec{k} \), by their analytical expression, the energy relation can be expressed in the following way:

\[ E_0 + E_0' + \sqrt{(E_0 - E_0')^2 + 12t^2 + 8\pi^2 \cos(\sqrt{3} k_x a_{SiC}) - 8\pi^2 \cos\left(\frac{\sqrt{3}}{2} k_x a_{SiC}\right)} \]  

\[ E(\vec{k}) = \frac{-8\pi^2 \cos\left(\frac{\sqrt{3}}{2} k_x a_{SiC} - \frac{\sqrt{3}}{2} k_y a_{SiC}\right)}{2} \]  

\[ \frac{1}{2} k_x a_{SiC} + \frac{\sqrt{3}}{2} k_y a_{SiC} \]  

(7)

Where \( E_0 = 3 \text{ eV} \) is the overlapping energy of neighbor carbon atoms, \( E_0' = 0.99 \text{ eV} \) refers to the interaction energy of Si–Si, \( t = 1.37 \text{ eV} \) is the nearest-neighbor C–Si interaction energy and the wave vector is considered as \( \vec{k} = k_x \hat{i} + k_y \hat{j} \). The wave functions have to satisfy boundary condition around the circumference of the scrolls [5]. In the presented relation, plus and minus signs (±) refer to the conduction and valence bands, respectively.

At this point, it is worth noting the difference between the boundary condition applied around the circumference of nanoscrolls and those used in the cases of nanoribbons (closed boundary conditions) and nanotubes (periodic boundary conditions). The periodic condition around the circumference of carbon nanotubes is naturally satisfied, because the start and the end of the chiral vector are coincided when rolling up a nanotube. The periodical boundary condition results in the quantized k-vectors perpendicular to the axes. Position and orientation of k lines near the K points in two-dimensional Brillouin zone (BZ) of graphene determine the energy dispersion relation of nanotubes [30]. If the quantization k lines pass through K points in the BZ, then a metallic nanotube with a zero band gap is formed. At the same time, if the K points are at (1/3) or (2/3) of the distance between two adjacent lines, then the nanotube shows semiconducting behaviour.

However, the periodic boundary condition of nanotube in circumferential direction becomes different for nanoribbons and nanoscrolls. Instead of a seamless tube-like cylinder, nanoribbons have two open boundaries. These open boundaries as well as the edge geometry condition can affect the electronic properties of nanoribbons. Actually, the linear combinations of dangling bonds at the edges form some eigenstates near the Fermi energy and determine the electronic properties of nanoribbons. Therefore, circumferential periodic boundary condition in nanotubes changes to the open boundary condition in nanoribbons [31]. On the other hand, nanoscrolls have spiral-like form with open edges at the ends and they do not have the same closed wound cylindrical structure as nanotubes. Therefore, it is assumed that the circumferential boundary condition will not be satisfied by nanoscrolls. A recent study by Chen et al [11] clearly demonstrates boundary condition of zigzag nanoscrolls. They noticed bond length variations in optimized nanoscroll structures which can induce band distortion. The distortion can be characterized as a result of boundary effect, interlayer interaction or \( \sigma-\pi \) rehybridization.

Considering only the effects of boundary condition, it is assumed that the boundary condition would not change the eigen states greatly and it only quantises k-vectors in a different manner. Therefore, the effect of boundary condition is considered as a K-space quantiser and the energy bands of nanoscrolls can still be studied from \( \pi \) and \( \pi^* \) energy bands of graphene layer. Through careful investigations, it is suggested that the quantization condition for \( \vec{K}, \vec{C} \) being only a phase shift from a multiple of \( \pi \) is a reasonable phenomenal approximation. Detailed comparison of the energy gaps of zigzag nanoscrolls and the corresponding nanotubes is presented in Chen et al’s work. Accordingly, \( \vec{K}, \vec{C} = 2\pi \theta - \varphi \) is presented as common boundary condition in nanoscrolls where \( \theta \) specifies the sub-band effect and \( \varphi \) is a special phase shift. Later, many interesting studies have been conducted regarding the electronic properties of nanoscrolls based on this developed boundary condition [22, 32].

Considering the presented energy band relation in equation (7) and the circumferential boundary condition for SiC nanoscrolls, a group of zigzag SiCNSs wrapped into the Archimedean spirals is studied. As is well known,
zigzag SiCNSs are formed by rolling up a SiC layer along the \( y \)-axis in the circumferential direction, i.e. they make a chiral angle of 0°. Based on the structural model of zigzag nanoscrolls \[10, 11\], the \( y \) component of the quantized momentum can be determined by:

\[
p_{Jy} = -k_{na} 2^{3/8} \sin \left( \frac{\pi}{2} \right)
\]

Substituting (8) into equation (7), we obtain the energy dispersion relation of zigzag SiCNSs:

\[
E_{Z}(k) = E_{0} + E'_{0} \pm \sqrt{(E_{0} - E'_{0})^{2} + 12t^{2} + 8t^{2} \cos \left( \frac{2\pi \theta - \varphi}{n} \right) - 16t^{2} \cos \left( \frac{2k_{x}a_{SiC}}{2} \right) \cos \left( \frac{2\pi \theta - \varphi}{2n} \right)}
\]

Where \( k_{x} \) refers to the magnitude of \( k \) along the axis of the nanoscroll, \( L \) is the length of spiral and \( n \) stands for the chirality. The developed energy relation for zigzag SiCNSs, equation (9), can be simplified by employing the Taylor expansion for cosine functions near the Fermi point as follows:

\[
E_{Z}(k) = E_{CO} + \sqrt{\frac{9\alpha}{16\sqrt{\beta}}}a_{SiC}^{2}k_{x}^{2}
\]

Where \( \alpha \) and \( \beta \) are given by \( \alpha = 8t^{2}(1 - (2\pi \theta - \varphi)^{2}/8n^{2}) \) and \( \beta = (E_{0} - E'_{0})^{2} + 4t^{2} - 2t^{2}(2\pi \theta - \varphi)^{2}/n^{2} \), respectively. Moreover, \( E_{CO} \) is defined by \( E_{CO} = 1/2(E_{0} + E'_{0} + \sqrt{\beta}) \). Here, the \( \varphi \) parameter stands for the phase shift introduced in the boundary condition of nanoscrolls and \( \theta \) is considered as \( \theta = 1, 2, \ldots, 2n \) which is defined as the number of sub-bands for a particular chirality. As proposed in in Chen et al’s work, inserting a special phase in the absolute periodic boundary condition of carbon nanotubes can provide a modified boundary condition appropriate for nanoscrolls. In accordance with the study of Chen et al the value of \( \varphi \) is fitted from the energy gap of a zigzag nanoscroll of type (16, 0). With the limitation of \( \varphi \) being positive and less than \( \pi, \varphi \) can be equated to 1.9242 or 2.2641 \[11\]. Accordingly, the band energy of a zigzag SiCNS near the Dirac point \( (k = 0) \) as a function of \( k \) is numerically plotted in figure 3.

In general, our numerical results suggests semiconducting behaviour for zigzag SiCNSs. In the parabolic part of the energy band structure, \( k_{x} \) can be written as follows:

\[
k_{x} = \frac{4\sqrt{3}}{3a_{SiC} \sqrt{\alpha}}(E_{Z} - E_{CO})^{1/2}
\]

Besides, considering the parabolic relation of the energy band structure for zigzag SiCNSs, one can find the corresponding effective electron mass, \( m^{*} \), as written below:
\[ m^* = \hbar^2 \left( \frac{d^2E_z}{dk^2} \right)^{-1} = \frac{8\hbar^2}{9\alpha_d_{\text{SiC}}^2} \]  

(12)

Where \( \hbar \) represents the reduced Planck’s constant or Dirac constant, in which \( \hbar \) equals \( h \) divided by \( 2\pi \) \((h = \hbar/2\pi)\). As mentioned before, it is necessary to derive the analytical expression of the density of states function to determine the intrinsic carrier concentration within a band. The density of states has a functional dependence on energy and indicates the number of allowed states per unit length at a given energy range as follows:

\[ \text{DoS} = \frac{\Delta n_i}{\Delta E_z} = \left( \frac{a_{\text{SiC}}}{\hbar^2 \beta^{3/4}} \right) \sqrt{\frac{m^*}{8\beta}} (E_z - E_{C0})^{-1/2} \]  

(13)

Figure 4 depicts DOS as a function of \( E \) for different values of chirality and the minimum sub-band index \((n)\). As it can be noticed, the DOS is directly dependent on the chirality \((n)\). Subsequently, using the Fermi–Dirac distribution function and the derived DOS function, we get the following expression for the intrinsic carrier concentration:

\[ n_i = \left( \frac{a_{\text{SiC}}}{\hbar^2 \beta^{3/4}} \right) \sqrt{\frac{m^*}{8\beta}} \int_0^\infty (E_z - E_{C0})^{-1/2} \frac{1}{1 + e^{x - \eta}} dE \]  

(14)

Considering \( x \) as the normalized energy, \( x = (E_z - E_{C0})/K_B T \), \( \eta \) as the normalized Fermi energy, \( \eta = (E_F - E_{C0})/K_B T \), multiplying the numerator and denominator of the derived expression by \( \sqrt{\pi} \) and defining the constant coefficient of the integral as \( A = \left( \frac{a_{\text{SiC}}}{\hbar^2 \beta^{3/4}} \right) \sqrt{\frac{m^*}{8\beta}} \), the following simplified expression is obtained for the carrier concentration:

\[ n_i = \frac{A(K_B T)^{1/2}}{\sqrt{\pi}} \frac{1}{1 + e^{-x - \eta}} \int_0^\infty x^{-1/2} \frac{1}{1 + e^{x - \eta}} dx \]  

(15)

The integral in equation (15) can be recognized as the gamma function, \( \Gamma \). \( \Gamma(j + 1) \) is defined as the gamma function of order \( j + 1 \), \( \Gamma(j + 1) = \int_{x=0}^{x=\infty} x^{j} e^{-x} dx \). It is also well-known that the gamma function at a non-integer argument equal to \( \frac{1}{2} \) becomes \( \sqrt{\pi} \). Finally, we arrive at the general following equation for the intrinsic carrier concentration of a zigzag SiCNS:

\[ n_i = N_C \Gamma_{-1/2}(\eta) \]  

(16)

Where \( N_C = \left( \frac{a_{\text{SiC}}}{\hbar^2 \beta^{3/4}} \right) \sqrt{\frac{m^*}{8\beta}} (K_B T)^{1/2} \) refers to the effective density of states and the gamma function, \( \Gamma_{-1/2}(\eta) \), is given by \( \Gamma_{-1/2}(\eta) = \frac{1}{\Gamma(\frac{1}{2})} \int_0^\infty \frac{x^{-1/2}}{1 + e^{x - \eta}} dx \).

As mentioned before, once the intrinsic carrier concentration of the SiCNSs is determined, we can explore the associated quantum capacitance near the charge neutral Dirac point using the second derivate of the total discrete energy spectrum.
carrier concentration relative to the states of energy. Meanwhile, based on the presented normalized energy in equation (15) as \( x = (E - E_{CB}) / k_B T \), the quantum capacitance can be equivalently written as:

\[
C_q = \frac{\partial Q}{\partial V} = \frac{e^2 \partial n_i}{\partial E} = \frac{e^2}{k_B T} \frac{\partial n_i}{\partial x}
\]

Consequently, the quantum capacitance for zigzag SiCNSs is determined as:

\[
C_q = \left( \frac{e^2 \alpha_{SSC}}{\hbar \beta^2} \right) \sqrt{\frac{m^*}{8 \beta k_B T}} \frac{x^{-1/2}}{1 + e^{x - \eta}}
\]

In the non-degenerate regime [33], the states in the conduction band are not fully filled at room temperature and only partially-filled band is presented. As a result, the ‘1’ in denominator of equation (18) becomes negligible compared with the exponential term. We can then express the final quantum capacitance in non-degenerate regime as follows:

\[
C_{q,\text{non-deg}} = \left( \frac{e^2 \alpha_{SSC}}{\hbar \beta^2} \right) \sqrt{\frac{m^*}{8 \beta k_B T}} \frac{x^{-1/2}}{1 + e^{x - \eta}}
\]

Though for the degenerate regime [33], the Fermi energy remains in the conduction band and the electron density is high so that \( f(E) \) approaches unity. This nearly complete filling of electron states up to the Fermi level suggests that the exponential term in denominator of equation (18) is about a value quite negligible compared to unity. Accordingly, the quantum capacitance of zigzag SiCNSs for the degenerate regime is given by:

\[
C_{q,\text{deg}} = \left( \frac{e^2 \alpha_{SSC}}{\hbar \beta^2} \right) \sqrt{\frac{m^*}{8 \beta k_B T}} \frac{x^{-1/2}}{1 + e^{x - \eta}}
\]

In Figure 5, we show our calculated quantum capacitance versus normalized energy, \( \eta \), for the general state and both non-degenerate and degenerate regimes using derived equations. For the degenerate regime, the zigzag SiCNS does not depend on \( \eta \) and it shows a constant value of quantum capacitance as high as \( 4.75 \times 10^{-11} \text{ F m}^{-1} \) (47.5 pF m\(^{-1}\)), while for non-degenerate regime it follows an exponential pattern. Besides, the quantum capacitance of a zigzag Si-doped CNS in the general state will undergo a significant rise as \( \eta \) increases for the range of \( 7 < \eta < 8 \). However, as the energy value rises beyond 8, the amount of the quantum capacitance stays constant and it is set to level off at approximately \( 4.75 \times 10^{-11} \text{ F m}^{-1} \) from \( \eta = 8 \) onwards. As a matter of fact, Figure 5 compares the dominancy of the quantum capacitance of SiCNSs at different levels of concentration. In degenerate regime the developed SiC scroll shows a considerable capacitance to have an effect or be important. This is due to the fact that the carrier concentration in the conduction band goes beyond its density of states.
The dominancy of the quantum capacitance which is attributed to the quantum confinement in nano-sized devices, can be clearly seen when analyzing the current–voltage characteristics of the device [34, 35]. Sub-threshold swing reduction and the ON current decreases, $I_{ON}$, are the main parameters that are significantly affected by the emergence of the quantum capacitance.

Furthermore, temperature dependence of the derived capacitance of zigzag SiCNSs is studied. Figure 6 illustrates the quantum capacitance variation in general state in function of normalized energy, $\eta$, for different temperature values. As the temperature is increased, more electrons acquire required energy to move to the conduction band and as a result more current flows. Thus, there will be a considerable rise in the carrier concentration by the temperature elevation. Accordingly, the quantum capacitance reaches the degenerate limit at lower normalized energy levels as the temperature increases. This effect is shown in figure 6 by the horizontal shift of the graph to the left as the temperature increases. In addition, the quantum capacitance is independent of temperature in the degenerate regime which is basically due to the fact that the carrier density is considerably high and the Fermi energy far outweigh the broadening parameter.

It is also worth pointing out that the results in the presented model in equations (13) to (20) are reported based on the proposed tight-binding model for the first sub-band of SiC nanoscrolls. Initially, the energy band structure of a single layer of silicon-doped graphene sheet is determined and then the energy dispersion relation of SiC nanoscrolls is obtained by applying the boundary condition of nanoscrolls to equation (7). The wave functions have to satisfy boundary condition around the circumference of the scrolls, $K_0 J_j = - K C$. Consequently, we arrive at equation (9) which determines the band energy of a SiCNS exclusively. It should be considered that the defined factors of $\alpha$, $\beta$ and $E_{CO}$ in the simplified form of the energy relation (equation (10)) and the following resultant formulas for the presented model (equations (11)–(20)) include chirality parameters of spirals. Afterwards, the density of state, carrier concentration and the quantum capacitance of SiC nanoscrolls are specifically developed for silicon doped nanoscrolls considering the derived parabolic relation of the energy band structure for zigzag SiCNSs in equation (10).

However, the presented analytical model of zigzag SiC nanoscrolls in equations (13) to (20) only describe the chirality dependence of electronic properties while the electronic behaviour of nanoscrolls are greatly related to their length. Thus, a similar approach for examining the effect of length on zigzag SiC nanoscroll properties is carried out and the analytical expression of energy band is derived again, but in terms of Archimedean spiral length. Considering the structural model of zigzag nanoscrolls and the boundary condition of nanoscrolls, $K_0 J_j = 2\pi \theta - \varphi$, we can obtain the $y$ component of the quantized momentum in terms of the spiral length:

$$k_y = \frac{2\pi \theta - \varphi}{L} \quad (21)$$

Inserting $k_y$ into the energy band dispersion relation of doped-graphene, the $E(k)$ relation for an $(n, 0)$ SiC nanoscroll is determined in terms of the spiral length. Following the same procedure of the presented analytical modelling as in equations (11) to (20), similar equations can be derived for the carrier concentration and
quantum capacitance of silicon doped carbon nanoscrolls, SiCNSs. Although the general representation of the new derived equations for carried concentration and the quantum capacitance in terms of spiral length are really the same as those presented in equations (14) to (18), the two parameters of $\alpha$ and $\beta$ are differently determined as

$$\alpha = 8t^2 (1 - 3a_{SiC} (2\pi \vartheta - \varphi) / 8L^2)$$

and

$$\beta = (E_0 - E_0')^2 + 4t^2 - 6t^2 a_{SiC} (2\pi \vartheta - \varphi)^2 / L^2,$$

respectively.

Figure 7 exhibits the intrinsic carrier concentration of zigzag SiCNSs as a function of $\eta$ (normalized Fermi energy) for several scroll lengths. From figure 7, it is realized that the carrier concentration, $n_i$, is proportional with the spiral length in reverse, in other words, the intrinsic carrier concentration of a zigzag SiCNS decreases as the spiral length grows up. Also, we see the same trend in ranging the length from 50 to 100. Subsequently, it can be concluded that the quantum capacitance of zigzag SiC nanoscrolls decreases when the spiral length increases.

3. Conclusion

Emergence of a new generation of high-technology nanomaterials continue to push forward the miniaturization of electronic devices and the improvement of their functionality. In parallel with device scaling, quantum confinement effects find a significant role in device performance. One of the most important class of nanostructures in terms of synthesis and practical application is SiC nanostructures whose outstanding properties provides a rich variety of applications for it. Moreover, it should be considered that SiC-based nanostructures have a main advantage that their integration into the current Si-based technology will be quite easier. In the presented study, many detailed analytical models have been established for some electronic characteristics of zigzag SiCNSs including the state density, carrier concentration and the quantum capacitance. Our studies demonstrate that the quantum capacitance of the studied zigzag SiCNSs reach degenerate limit at approximately of $4.75 \times 10^{-11}$ F m$^{-1}$ (47.5 pF m$^{-1}$). Moreover, the effects of spiral structure such as length and chirality on the density of state and carrier concentration of zigzag SiCNSs was investigated.

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