Chapter

Graphene-Based Nanophotonic Devices

Ankur Pandya, Vishal Sorathiya and Sunil Lavadiya

Abstract

Graphene is an ideal 2D material that breaks the fundamental properties of size and speed limits by photonics and electronics, respectively. Graphene is also an ideal material for bridging electronic and photonic devices. Graphene offers several functions of modulation, emission, signal transmission, and detection of wideband and short band infrared frequency spectrum. Graphene has improved human life in multiple ways of low-cost display devices and touchscreen structures, energy harvesting devices (solar cells), optical communication components (modulator, polarizer, detector, laser generation). There is numerous literature is available on graphene synthesis, properties, devices, and applications. However, the main interest among the scientist, researchers, and students to start with the numerical and computational process for the graphene-based nanophotonic devices. This chapter also includes the examples of graphene applications in optoelectronics devices, P-N junction diodes, photodiode structure which are fundamental devices for the solar cell and the optical modulation.

Keywords: Graphene, PN diode, photodetector, modulator, transistor

1. Introduction

The scientific community across the globe considered graphene as one of the most revolutionary 2D nanomaterials of the world that possesses zero energy bandgap [1]. As shown in **Figure 1**, being the monoatomic carbon layer arranged in a honeycomb lattice, graphene possesses unique attractive properties and by the virtue of which it has attracted strong scientific and technological interests [2–5]. Graphene has shown great application potential in many fields, such as nanoelectronics [5, 6], energy storage devices [6–10] and bioelectronic device applications [11–13]. The linear dispersion relation in graphene at the ends of the First Brillouin Zone is shown in **Figure 2** according to which the bandgap at the Dirac point is zero. However, zero energy bandgap limits the applications of pristine graphene on a wide-scale especially in graphene-based nanoelectronics because, in the absence of energy bandgap, it is not possible for pristine graphene-based electronic devices to be operated in ON and OFF states which is desirable for logic gate circuits. To overcome such limitations of pristine graphene and to improve its applicability for designing nanoelectronic devices, the interest also builds up towards the study on doped graphene. Suitable doping with proper concentration can introduce the desired bandgap in graphene that enables graphene to be utilized in electronic circuits at the nanoscale. It has been reported that the hydrogen passivated armchair GNR exhibits direct bandgap at the edges [14]. Moreover, the bandgap can be introduced and tuned by transforming

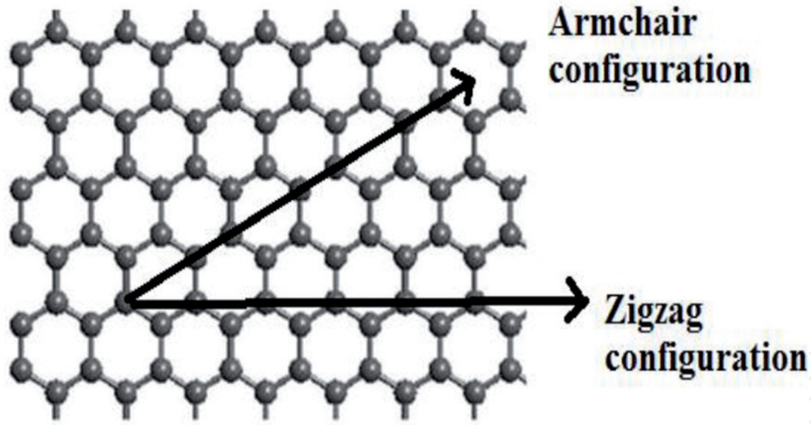

Figure 1.
Monolayer graphene nanoribbon [17].

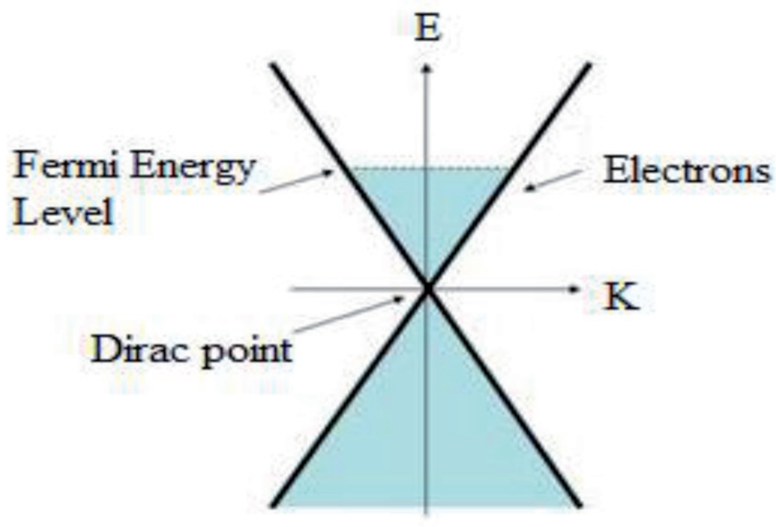

Figure 2.
The linear dispersion relation in graphene at the ends of First Brillouin Zone [18].

graphene sheet into its nanoribbon form of finite width i.e. graphene nanoribbon (GNR) [15, 16]. However, the bandgap of graphene nanoribbons shows different magnitudes for three groups i.e. Na =3p, 3p + 1, and 3p + 2 where Na is the number of dimers and p is an integer [15]. The magnitude of bandgap oscillates between these three groups with the number of dimers (N) i.e. $E_{g(3p+1)} > E_{g(3p)} > E_{g(3p+2)}$. The energy band gap of armchair GNR is determined as a function of the number of dimers wherein the smaller the number of dimer lines, the smaller the nanoribbon width and hence higher the bandgap [15].

The GNRs are narrow strips of graphene nanosheet of finite width possessing structural similarity to that of unrolled carbon nanotube (CNT). GNRs possess mainly two types of structural configurations termed as armchair graphene nanoribbon (A-GNR) and zigzag graphene nanoribbon (Z-GNR). A-GNRs exhibit semiconducting properties whereas Z-GNRs are metallic in nature [15]. This behavior exclusively depends on how the graphene sheet cuts along with its plane (**Figure 1**). As shown in **Figure 3**, the bandgap increases with reducing nanoribbon width in an exponential manner [17–20]. Recently, it has been reported that applying a transverse magnetic field to the ribbon width induce the tunable bandgap i.e. tuning of the bandgap is possible by changing the magnitude of the applied

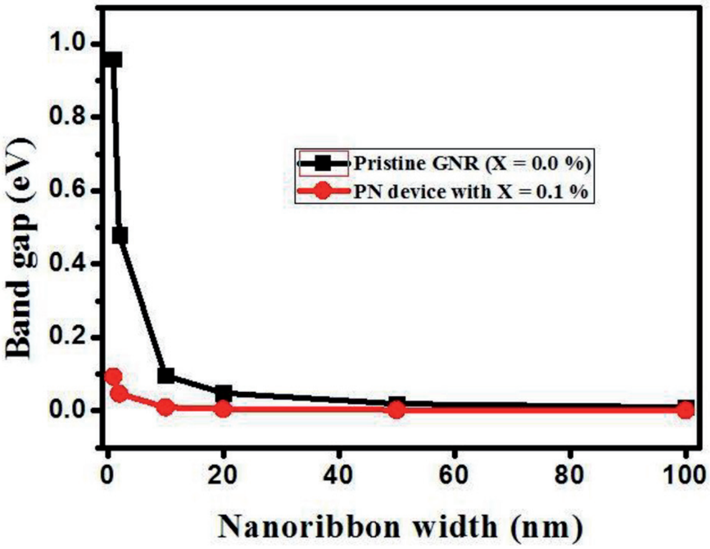

Figure 3.
The energy bandgap varies with nanoribbon width and doping concentration [17].

magnetic field [21]. The important aspect of a variable bandgap of a material is to develop efficient and flexible optoelectronic devices and sensors that work with the utmost accuracy. Considering this background, the subsequent sections discuss the photonic devices at the nanoscale in the present chapter.

2. Photonic devices at nanoscale

Photonic devices are the components that generate or detect the photonic flux that is developed and utilized for either electronic signal or light. The P-N device in the form of a light-emitting diode, photovoltaic cell, and the laser device is the most common type of photonic device. Traditionally these devices are designed and fabricated using Si or Ge due to which limited efficiency, broad bandwidth, high power consumption are few of the major limitations of current electronic devices. These limitations may be overcome by developing the replica of current electronic components at the nanoscale. The main theme of devices at the nanoscale is the smaller the dimensions, the lesser the power consumption, and the higher the efficiency. As mentioned above, though graphene possesses a zero energy bandgap in its nanosheet form, it exhibits a finite bandgap in its nanoribbons form which varies with the width of the nanoribbon. **Figure 3** shows that the bandgap of pristine graphene reduces exponentially with the increase in nanoribbon width.

It is possible to further enhance electronic transport properties of GNR with dopant adatoms [22–26] – that may help to fabricate graphene-based P-N nanodevices [27] as well as the surface acoustic wave sensors [28] at nanoscale. Moreover, it has also been proposed by several research groups that the doping of boron and nitrogen in graphene exhibits the possibility of engineering the graphene-based p-n junction at nanoscale as well as graphene aerogels for oxygen electro-catalysis [29, 30] wherein boron being trivalent and nitrogen being pentavalent impurities introduce the energy bandgap. **Figure 4** shows the boron and nitrogen-doped graphene nanoribbon based forward-biased p-n device. First-principles quantum transport calculations of electronic properties of boron and nitrogen-doped armchair GNR showed that the B-doped p-type GNR based device can exhibit high levels of performance, with high ON/OFF ratios and low subthreshold swing [31].

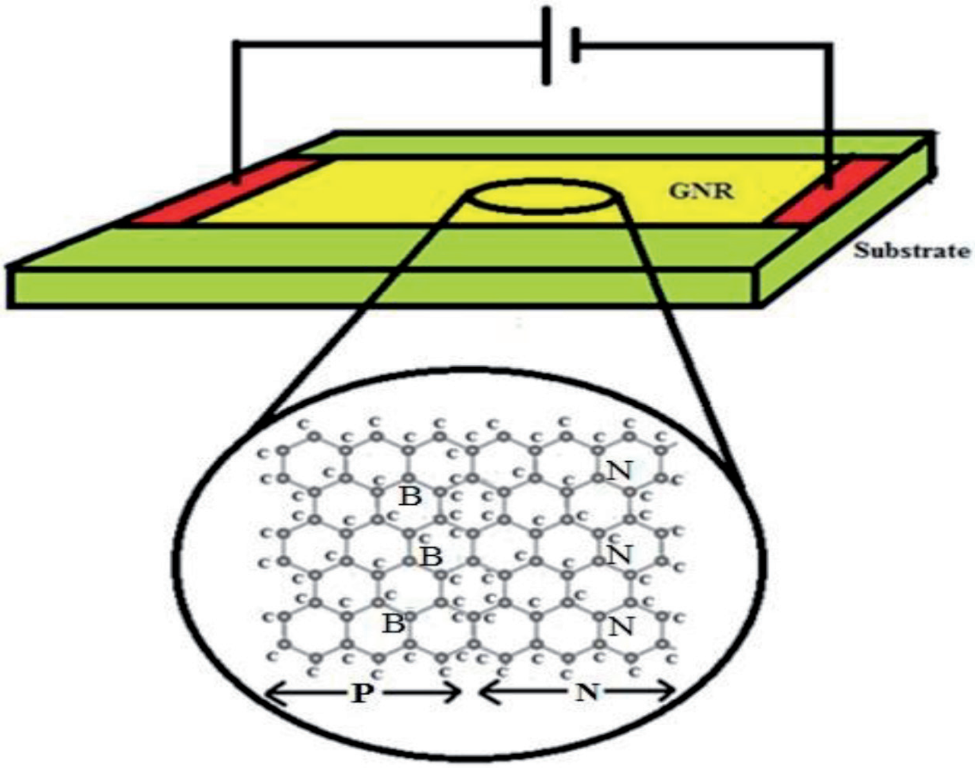

Figure 4.
Graphene-based P-N device [17].

2.1 Graphene-based P-N device and field effect transistor

The P-N device is one of the fundamental devices of an electronic circuit that controls the charge carrier (electron) current in the circuit manufactured from semiconducting materials such as silicon (Si) and germanium (Ge). It has a positive (p) region and negative (n) region created via doping semiconductor material by trivalent and pentavalent impurities respectively. Since AGNR exhibits semiconducting properties it is possible to design P-N device at the nanoscale using AGNR configuration. This type of P-N device will be having better electronic transport properties compared to traditional one because armchair graphene is not only a semiconductor but transparent and flexible also due to which it can be placed in nanoelectronic circuit. In addition to this, according to the recent article on graphene-based terahertz frequency detection, it is possible to design and fabricate graphene p-n junction based nano-antenna (bolometer) using the photo-thermoelectric effect wherein it is reported that with the dual gated dipolar antenna of the gap of 100 nm it is possible to concentrate the incident radiation for better photoresponse [32]. Graphene based field-effect transistors (GFET) are being investigated for more than a decade [33, 34].

There are several reasons behind this hunt such as limited electronic transport parameters of current electronics materials (Si, Ge) i.e. electron mobility and hence conductivity, poor heat dissipation rate of Si and Ge, and their tensile strength, failure of Moore's law, etc. In this context, graphene possesses superiority among all the materials known to researchers because graphene exhibits better electrical, mechanical, thermal, and optical properties in comparison with Si and Ge which are listed as follows: electrical conductivity of graphene is 10^7 S/m [35] whereas for Si it is 10^3 S/m, the electrical mobility of graphene is 10^5 cm^2/Vs [36] whereas for Si it is 10^3 cm^2/Vs, and 4×10^3 cm^2/Vs for Ge, Young's modulus of graphene is around 1.2 TPa [37] whereas that for both Si and Ge is 1 MPa, the thermal conductivity of graphene is around 5000 W/mK [37] whereas it is 1300 W/mK for Si and

580 W/mK for Ge. Considering these values of various parameters, it is obvious that graphene as a material is far better than the traditional semiconductors Si and Ge. In addition to this, graphene is a flexible transparent conducting thin film, unlike Si and Ge, due to which graphene can be used to develop flexible and transparent electronic devices that are base of wearable electronics [37].

The field effect transistor (FET) is one of the most important and fundamental electronic device that uses electric field to control the current and possesses three electrodes source, drain, and gate. A semiconductor channel is connecting source and drain and the third one i.e. gate controls the current. Implementation of graphene field effect transistors (GFET) in sensors has large number of benefits over the bulk FET made from Si. As the silicon is bulk semiconductor, the charge carriers at the channel interface have difficulty to penetrate into the device which limits response sensitivity of the device. On the other hand, as the graphene possesses two dimensional structure, the sensitive channel is itself the surface that ultimately improves the surface sensitivity. In addition to this, the carrier scattering rate through graphene is much lower than that in the case of bulk semiconductors. Therefore, the carrier energy loss also much lower than that for the bulk semiconductors. The fabrication of GFET is possible on Si/SiO_2 substrate with metal contacts via chemical vapor deposition (CVD) technique. G. Fiori et al. explored the possibility of tunable gap GFET considering bandgap opening by applying vertical electric field and using atomistic simulations based on the self-consistent solution of the Poisson and Schrödinger equations within the non-equilibrium Green's function formalism [38]. The chemical and biological sensors based on GFET were investigated to show their sensitivity towards detection of protein of different charge types [39]. Such sensors are having relatively higher sensitivities for biomolecules. On the other hand, GFET based high temperature sensor has been reported that works up to 600°C with utmost accuracy wherein researchers calculated the resistivity of the device using semi-classical transport Equations [40]. Graphene succeeded to implant itself in the broad field of organic light emitting diode (OLED) which is one of the important parts of optoelectronics [41–43]. Traditional OLEDs have their applications in screens of computer, mobile phones and cameras. In general, indium tin oxide (ITO) is used as transparent conductive thin film which is brittle and not flexible. In addition to this, indium may diffuse into active layers of OLEDs [44]. These limitations may be overcome using graphene instead of ITO because the work function of both the materials is same (4.5 eV).

2.2 Graphene-based photodetector and photovoltaic devices

Photodetectors are significant optoelectronic devices that detect the optical flux by converting the absorbed optical energy into the electronic current. They are part of remote control, televisions and DVD players. The spectrum responded by detectors is entirely depends on the bandgap of the material of detector. The traditional photodetectors consist of IV or III-IV semiconducting materials that are suffering from long-wavelength limits because these materials do not respond to the optical energy if its energy is less than the bandgap. Hence, the particular material becomes transparent for that radiation. As a solution of this problem, the implementation of graphene is the better option as graphene absorbs from ultraviolet to terahertz range [45, 46]. Since, the response time of a photodetector depends on the carrier mobility, graphene based photodetectors (GPDs) can be ultrafast because graphene exhibits very high carrier mobility. It is also possible to utilize photo-thermoelectric effect for efficient GPDs. In photo-thermoelectric effect, the photon energy converts into the heat followed by photocurrent generation. This is an important attribute to the fields of graphene based optoelectronics, photo-thermocouple devices and photovoltaic applications [47].

Graphene based touch screen is an emerging field as well because graphene is transparent and conducting too. This is the reason why graphene transparent conducting films (GTCFs) are promising layers for touch screens of electronic device displays. Graphene being mechanically strong, with high chemical durability, non-toxic, and cheap is one of the ideal materials for displays. Traditional displays consist of ITO which is costly, wear-resistant, brittle and has limited chemical durability. Graphene-based touch panel display can be grown by screen printing by the CVD technique [48]. Thus, GTCF may be an important part of future flexible and efficient touch screens.

For decades, it is known to us that photovoltaic (PV) cells convert light into electricity which is the main theme of traditional solar panels that are using silicon (Si) or germanium (Ge). The energy conversion efficiency of these materials is limited to around 25% [49]. Moreover, since Si and Ge are not flexible materials it limits the flexible solar cells or panels which are important components of futuristic wearable electronics. These limitations can be overcome by using graphene-based PV cells for this aspect. Graphene plays multiple roles in a photovoltaic cell i.e. photoactive material, transparent as well as conducting (TC) layer, charge transport layer, and catalyst. Among all these exciting and promising applications of graphene, the terahertz (THz) photonics based on graphene is a promising field of research as well which is capable to develop high-performance terahertz devices operated in the region between 300 GHz to 10 THz. at 300 K [50].

3. Graphene-based metamaterial

The modern form of artificial substance Metamaterials (MMs) has recently been examined for their electromagnetic properties that are missing in typical natural materials [51, 52]. The different results such as negative refractive index [53], perfect lensing [54], bolometer [55] etc. are discovered when utilizing these properties. From the other horizon, owing to its exceptional electrical, electronics and optical properties, such as strong thermal power, wide carrier mobility, and extremely young module [56], have acquired considerable attention in the domain of the thin and lightweight metamaterial research. Graphene is a 2-dimensional, radioactive medium that offers electrical and optical control across a large spectrum of frequencies, such as THz [57–59] and GHz [60]. The graphene's conductivity can be managed by various parameters such as temperature, duration, dispersion rate, and chemical potential [58]. Several devices are suggested for complete absorption [59, 61–63] polarization-insensitive [64–67], broad-angle [64–68], tunability [69–72]. For the Terahertz area and the Microwave, others are examined. **Figure 5** shows the example of the graphene-based squared shaped spiral metamaterial design for the polarization application. It is very much essential to discuss the refractive index parameters to identify the effect of metamaterial and negative refraction. The effective refractive index parameters can be identified by considering the transmittance and reflectance values of any two-port devices. The negative index behavior of any structure realized the overall effect of the metamaterial at a specific resonance frequency. The Schematic shown in **Figure 5** was numerically investigated to identify the reflection and transmission behavior of the THz wave. According to the results of transmittance and reflectance values, the effective refractive index was calculated for the band of 1 THz to 3 THz frequency region using the mathematical formula given in [73]. The negative refractive index response of the structure has been shown in **Figure 6**. **Figure 6** was derived for the different modes of excitation applied to the structure as shown in **Figure 5**. The effective refractive index of the normal and complimentary structure shows that the metamaterial effect was observed at the different resonance points for range 1 THz to 3 THz range. The proposed metamaterial

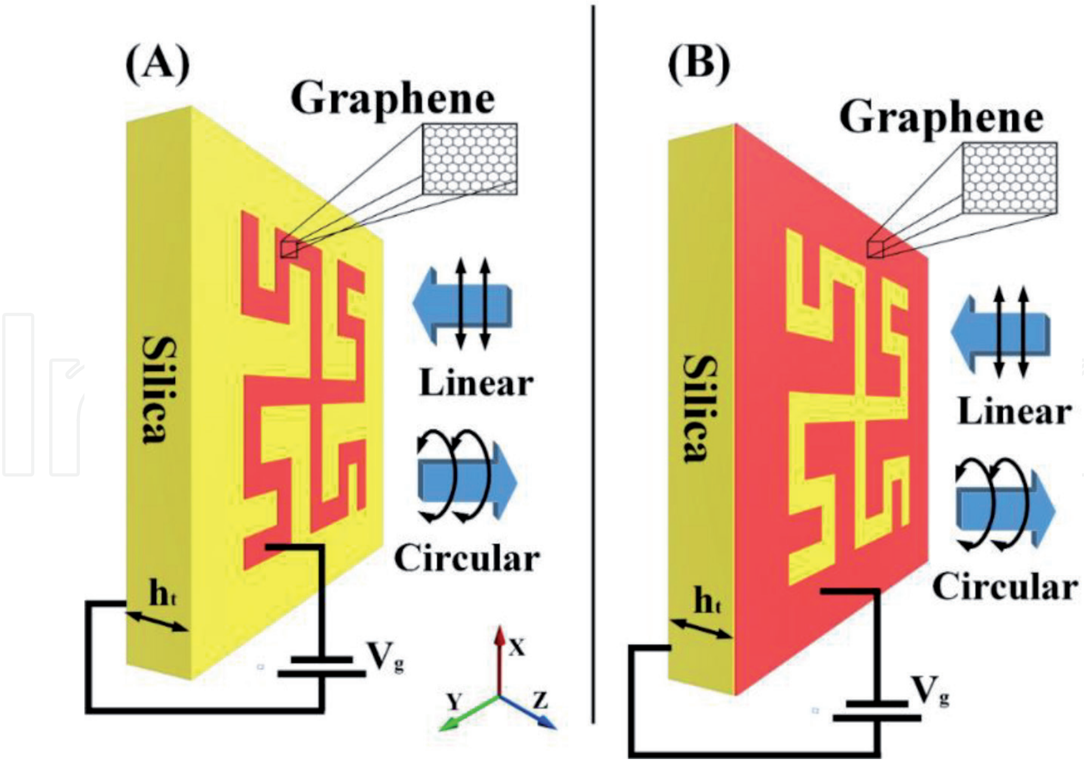

Figure 5.
Schematic of the squared spiral-shaped graphene metamaterial structure. (A) 3D view of the squared spiral-shaped graphene normal structure (SSSG – N), (B) squared spiral-shaped graphene complementary structure (SSSG – C) [73].

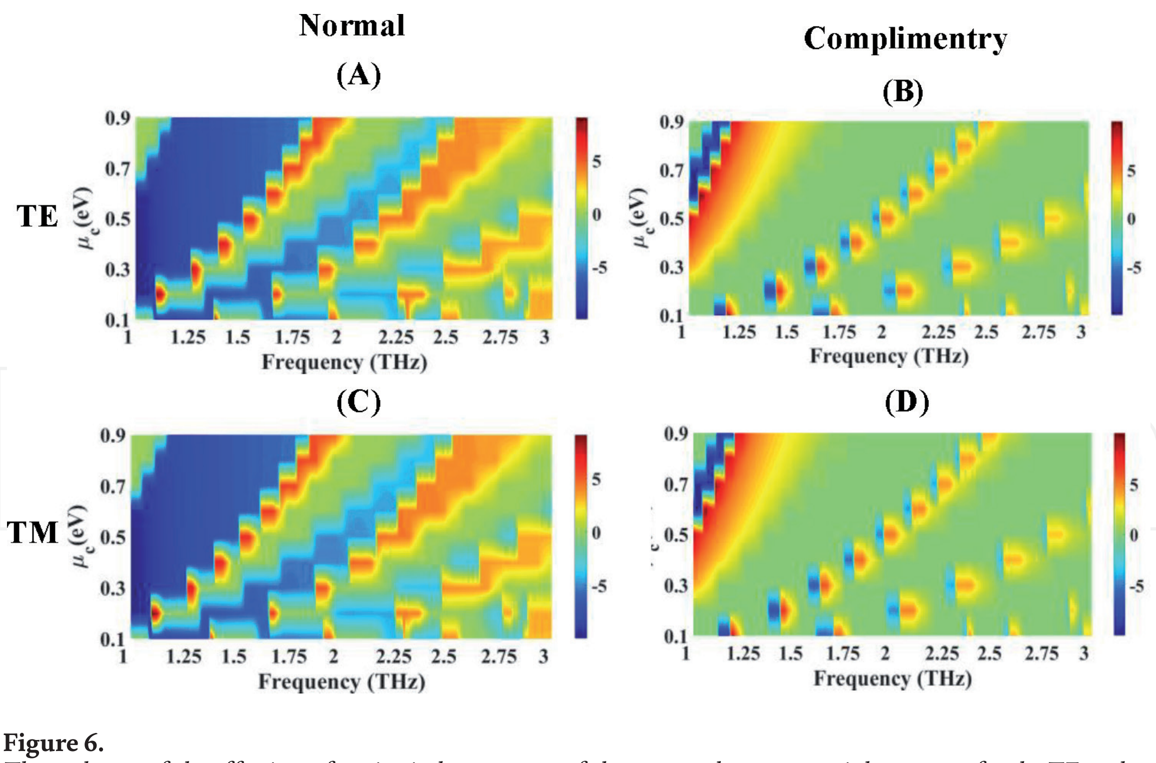

Figure 6.
The real part of the effective refractive index response of the proposed metamaterial structure for the TE and TM mode of the excitation over 1 THz to 3 THz frequency (structure shown in ***Figure** 5*). The response is derived for the different chemical potential varied from 0.1 eV to 0.9 eV. (A) SSSG – N with TE excited mode, (B) SSSG – C with TE excited mode, (C) SSSG – N with TM excited mode and (D) SSSG – C with TM excited mode [74].*

behavior can help with different applications such as absorber, polarizer, superlens, etc. **Figure 6** also shows that for the different mode of the excitation (TE or TM) does not affect to the resonance behavior due to the squared spiral symmetric structure of the top graphene layer as shown in **Figure 5**.

4. Graphene surface conductivity model

Graphene-based photonics devices need to be analyzed by the specific mathematical characteristic before implementing it to the fabrication stage. It is important to identify the behavior of the graphene for the different external parameters such as temperature, frequency, external potential. Graphene can be modeled as one atom thick infinitesimally thin and two-sided surface. This model of the graphene can characterize by the surface conductivity model. Complex permittivity of the graphene sheet [75] is expressed by $\varepsilon(\omega)$ as expressed in Eq. 1, where the conductivity of the graphene σ_s expressed from Kubo formula as mentioned in Eqs. (2)–(4) [76]. Graphene conductivity is depending on the various parameters such as temperature, scattering rate, frequency and external chemical potential.

$$\varepsilon(\omega) = 1 + \frac{\sigma_s}{\varepsilon_0 \omega \Delta} \tag{1}$$

$$\sigma_{intra} = \frac{-je^2 k_B T}{\pi \hbar^2 (\omega - j2\Gamma)} \left(\frac{\mu_c}{k_B T} + 2\ln\left(e^{-\frac{\mu_c}{k_B T}} + 1 \right) \right) \tag{2}$$

$$\sigma_{inter} = \frac{-je^2}{4\pi\hbar} \ln\left(\frac{2|\mu_c| - (\omega - j2\Gamma)\hbar}{2|\mu_c| + (\omega - j2\Gamma)\hbar} \right) \tag{3}$$

$$\sigma_s = \sigma_{inter} + \sigma_{intra} \tag{4}$$

Here, ε_0 is the vacuum permittivity, σ_s is the monolayer conductivity, e is the fundamental electron charge value, ω is angular frequency, k_B is the Boltzmann's constant and $\hbar$ is the reduced Planck's constant. In this work, the chemical potential of graphene μ_c is varied between 0.1 eV to 0.6 eV, electron relaxation time τ^{-1} = 10-13 s, Γ is phenomenological scattering rate, graphene sheet thickness Δ = 0.34 nm and temperature T = 300 K. Carrier concentration of the whole graphene sheet will be controlled by field-effect, which can be indicated as: $n_s = \varepsilon_0 \varepsilon_d V_g / et_d$ [77], where ε_0, ε_d = 2.25 and td = 2 μm are free space permittivity, permittivity of silica and thickness of silica layer respectively. Vg is gate voltage applied to graphene surface. Many research works have been used the graphene conductivity formula as it is easy to define in the computational studies with finite element method (FEM) of finite difference time domain method (FDTD). Simplified graphene conductivity module can be used also to identify the behavior of the entire structure for different physical parameters. It is also available several software packages that help the researchers to characterize the graphene material using mathematical modeling. RF module of the COMSOL Multiphysics provides the 2D and 3D analysis of the graphene-based devices for the photonics applications [77–79].

5. Conclusion

In summary, the present chapter discusses the current and future possibilities to incorporate wonder material graphene into the current photonic devices to enhance their performance in terms of efficiency, and sensitivity of sensors at the nanoscale replacing traditional semiconductors by graphene. Being a flexible, optically transparent, electrically as well as thermally conducting nanomaterial, graphene, in its nanosheet and nanoribbons forms, can be implanted into the current optoelectronic devices to overcome their existing limitations. However, the synthesis and insertion of graphene and its allotropes into the devices require state-of-the-art and is challenging too. We propose that the inclusion of graphene in traditional devices will take the current electronic devices to new horizons and will open up new frontiers of optoelectronic sensor technologies.

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