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Propagation of Surface Waves Along the Graphene Coated Metal Cylindrical Waveguide Embedded in Dielectric Environment

Mariam Saeed[a], Abdul Ghaffar[a*], Muhammad Yasin Naz[a] and Muhammad Asif Hanif[b]

[a]Department of Physics, University of Agriculture, Faisalabad, Pakistan

[b]Department of Chemistry, University of Agriculture, Faisalabad, Pakistan

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Abstract. A theoretical formulation is developed for the graphene coated metallic cylindrical waveguide embedded in dielectric environment. The graphene coating is considered to be infinitesimally thin and its conductivity is modeled in the framework of Kubo's formulism. The dispersion relation for the fundamental transverse magnetic plasmon modes propagating at the metal-graphene dielectric interface is derived using Maxwell's equations and impedance matching boundary conditions. It is demonstrated that propagation characteristics of surface waves are sensitive to various parameters and can be modulated by altering chemical potential of graphene and refractive index of the surrounding environment. The reduction of normalized propagation constant by increasing the diameter of the metallic cylinder revealed the potential applications of proposed structure for the designing of miniaturized inter connect for optical circuit. This work may enrich the electro-magnetic theory which is of great importance for various optoelectronic applications.

Keywords: graphene, dielectric environment, optoelectronic.

Introduction

Surface plasmon polaritons are evanescent waves propagating at the metal-dielectric interface due to the coupling of the free electron oscillations with light photons (Maier, 2007). The propagation characteristics of the SPPs depend upon the properties of the materials constituting the waveguide. The wide range of applications of surface waves in communication, sensing, spectroscopy, integrated circuit designing and miniaturization of optoelectronic devices has gained the attention of scientific community since last two decades (Engel *et al*., 2014; Sorger *et al*., 2012; Anker *et al*., 2010). To achieve strong field confinement, low propagation losses with long propagation length of surface waves in THz (far infrared and infrared) frequency regime is the main goal of the various research groups. Planar and circular waveguides with different compositions such as dielectric, metal, metamaterials, plasma and chiral materials etc. have been investigated extensively in this regard (Yaqoob *et al.*, 2018; Ghosh and Kakade, 2012; Hanson, 2008). Since the experimental realization of isolated graphene sheets by Geim, the quest for the controlled and tunable surface waves attained a new direction exploiting a new area of research named as graphene plasmonics (Geim, 2011).

*Author for correspondence; E-mail:aghaffarr16@uaf.edu.pk

Graphene, one atom thick allotrope of carbon, due to its zero band gap and extraordinary chemical, physical and electrical properties provides an additional degree of freedom to gain active control over the propagation and modulation of surface waves for optical sensing, biochemical sensing, THz communication and THz spectroscopy applications (Huang *et al.*, 2016; Liu *et al.*, 2012). The conductivity of the graphene which is responsible for providing tunability of surface waves is represented by Kubo' formulism. It is comprised of inter band and intra band conduction as shown in the equation:

$$\sigma_g(\omega,\mu_c,\tau,T) = j\,\frac{e^2 K_B T}{\pi\hbar^2(\omega+\frac{j}{\tau})}\left(\frac{\mu}{K_B T} + 2Log\left[e^{-\frac{\mu}{K_B T}}+1\right]\right)$$

$$+\, j\,\frac{e^2}{4\pi\hbar^2} Log\left[\frac{2|\mu|+\hbar^2(\omega+\frac{j}{\tau})}{2|\mu|+\hbar^2(\omega+\frac{j}{\tau})}\right] \qquad (1)$$

This equation indicates that graphene conductivity is highly sensitive to optical frequency (ω), chemical potential (μ_c), scattering rate of carrier concentration (τ) and Temperature (T) (Yaqoob *et al.*, 2019). The investigation of the different graphene based structures such as planar structures, graphene ribbons, graphene coaxial cylindrical waveguides and graphene shutters revealed different types of strongly confined modes with low loss propagation compared to ordinary metal-dielectric SPP waves under different frequency ranges (Yaqoob *et al*., 2019; Gric and Hess, 2017; Kuzmin *et al*., 2016; Fei *et al*., 2015; Vakil and Engheta, 2011). Numerous studies based on metal dielectric exhibit strong mode confinement but great propagation losses as well. The authors in (Kotelnikov and Stupakov, 2015) computed a dispersion relation for SPPs travelling along the interface of cylindrical metal waveguide embedded in dielectric medium. Dispersive behaviour and modulation of surface waves demonstrated a high gain and stronger field confinement exceeding 90% for 250 nm thick silver-GaAs nanowire, enabling it an ideal interconnect for nanophotonic circuitry (Handapangoda *et al*., 2010). The multimode plasmon modes were found to be propagating in metallized, capillary waveguides designed for sensing applications (Buric *et al*., 2010). The excitation and manipulation of dynamically tunable hybrid surface waves at chiral-graphene metal interface of a planar waveguide was reported in (Yaqoob *et al*., 2018).

In this pursuit, a graphene coated metal cylindrical waveguide embedded in dielectric environment is presented to investigate the propagation characteristics of SPPs at graphene metal interface. The details of the mathematical formulation of the plasmon modes propagating along the metal graphene dielectric (MGD) interface is provided in section 2. Section 3 contains the detailed analysis of dispersion curve based on numerical simulations in terms of normalized propagation constant and normalized frequency. The impact of various geometrical, graphene and dielectric parameters on the dispersive behaviour of the surface waves is also discussed in this section. In the end, the conclusions are presented.

Material and Methods

The cylindrical waveguide composed of gold nanowire coated with infinitesimally thin (0.35 nm) graphene sheet embedded in an isotropic dielectric medium is proposed. The ε_m and μ_m is considered as permittivity and permeability of the metal. However, the permittivity and permeability of dielectric medium is taken as ε_d and μ_d as shown in Fig. 1. The radius of the cylinder is R.

The propagation of the surface waves moving along the z-axis due to the cylindrical symmetry of the structure is governed by the solution of Maxwell equations in cylindrical co-ordinates along with boundary conditions in each region. The time dependence is considered as $e^{j\omega t}$ in all formulations. For the core region where $\rho<R$ Electric and magnetic fields are as follows:

$$E_z^1 = A_m I_m(\gamma_1\rho) exp(jm\varphi) exp(j\beta z) \qquad (2)$$

$$E_\varphi^1 = \frac{j}{-\gamma_1^2}\left\{\frac{jm\beta}{\rho} A_m I_m(\gamma_1\rho) - \omega\mu_m B_m \gamma_1 I_m'(\gamma_1\rho)\right\} exp(jm\varphi)\, exp(j\beta z) \qquad (3)$$

$$E_\rho^1 = \frac{j}{-\gamma_1^2}\left\{\beta A_m \gamma_1 I_m'(\gamma_1\rho) + \frac{jm\omega\mu_m}{\rho} B_m I_m(\gamma_1\rho)\right\} exp(jm\varphi)\, exp(j\beta z) \qquad (4)$$

$$H_z^1 = B_m I_m(\gamma_1\rho) exp(jm\varphi)\, exp(j\beta z) \qquad (5)$$

$$H_\varphi^1 = \frac{j}{-\gamma_1^2}\left\{\frac{jm\beta}{\rho} B_m I_m(\gamma_1\rho) + \omega\varepsilon_m A_m \gamma_1 I_m'(\gamma_1\rho)\right\} exp(jm\varphi)\, exp(j\beta z) \qquad (6)$$

$$H_\rho^1 = \frac{j}{-\gamma_1^2}\left\{\beta B_m \gamma_1 I_m'(\gamma_1\rho) - \frac{jm\omega\mu_m}{\rho} A_m I_m(\gamma_1\rho)\right\} exp(jm\varphi)\, exp(j\beta z) \qquad (7)$$

where;
ω = incident frequency; $\gamma_1 = \sqrt{(\beta^2 - k_m^2)}$ is decay constant; β is wave vector and $I_m(\gamma_1\rho)$ is modified Bessel function of first kind, where (m=0,1,2,……)

$k_m^2 = k_o^2(\varepsilon_m\mu_m)$, $k_o = \omega\sqrt{(\varepsilon_0\mu_0)}$, A_m and B_m are unknown constants (Saeed *et al*., 2020).

For the outer region where $\rho > R$ electromagnetic field equations takes the form as follows:

$$E_z^2 = C_m K_m(\gamma_2\rho) exp(jm\varphi) exp(j\beta z) \qquad (8)$$

$$E_\varphi^2 = \frac{j}{-\gamma_2^2}\left\{\frac{jm\beta}{\rho} C_m K_m(\gamma_2\rho) - \omega\mu_d D_m \gamma_2 K_m'(\gamma_2\rho)\right\} exp(jm\varphi)\, exp(j\beta z) \qquad (9)$$

$$E_\rho^2 = \frac{j}{-\gamma_2^2}\left\{\beta C_m \gamma_2 K_m'(\gamma_2\rho) + \frac{jm\omega\mu_d}{\rho} D_m K_m(\gamma_2\rho)\right\} exp(jm\varphi)\, exp(j\beta z) \qquad (10)$$

$$H_z^2 = D_m K_m(\gamma_2\rho) exp(jm\varphi) exp(j\beta z) \qquad (11)$$

$$H_\varphi^2 = \frac{j}{-\gamma_2^2}\left\{\frac{jm\beta}{\rho} D_m K_m(\gamma_2\rho) + \omega\varepsilon_d C_m \gamma_2 K_m'(\gamma_2\rho)\right\} exp(jm\varphi)\, exp(j\beta z) \qquad (12)$$

$$H_\rho^2 = \frac{j}{-\gamma_2^2}\left\{\beta D_m \gamma_2 K_m'(\gamma_2\rho) - \frac{jm\omega\mu_d}{\rho} C_m K_m(\gamma_2\rho)\right\} exp(jm\varphi)\, exp(j\beta z) \qquad (13)$$

where;

ω=incident frequency; $\gamma_2=\sqrt{(\beta^2-k_2^2)}$ is decay constant; β is wave vector and $K_m(\gamma_2\rho)$ is modified Bessel function of second kind, where (m=0,1,2,……)

$k_2^2=k_o^2\,(\varepsilon_d\mu_d)$, $k_o=\omega\sqrt{(\varepsilon_0\mu_0)}$, C_m and D_m are unknown constants.

For brevity, the phase factor *exp* ($j\beta z+jm\rho-j\omega t$) is omitted in the expressions of electromagnetic fields, the real part of β representing phase constant is always larger than the wave vector of EM wave, so SPPs modes are surface waves decaying away from the graphene layer. Its imaginary part is the attenuation constant representing propagation loss in the z direction. The *m* represents the order of SPPs mode. The *m*=0 mode is the fundamental TM mode which has three fields components E_z, E_r, H_φ.

Plasmon modes at ρ=R are originated due to the surface conductivity σ_g of graphene which is characterized by Kubo formula. The impedance boundary conditions approach is utilized to model the tangential components of EM field on the interface of metal graphene dielectric.

$E_Z^1=E_Z^2$, $E_\varphi^1=E_\varphi^2$, $H_Z^2-H_Z^1=-\sigma_g E_\varphi^1$ and $H_\varphi^2-H_\varphi^1=-\sigma_g E_Z^1$

By employing the equations into the boundary conditions, the Eigen equation for the m-th order mode can be presented as:

$$\begin{vmatrix} I_m(\gamma_1 R) & 0 & -K_m(\gamma_2 R) & 0 \\ \frac{jm\beta}{-\gamma_1^2 R} I_m(\gamma_1 R) & \frac{\omega\mu_m}{\gamma_1} I'_m(\gamma_1 R) & \frac{jm\beta}{\gamma_2^2 R} K_m(\gamma_2 R) & -\frac{\omega\mu_m}{\gamma_1} K'_m(\gamma_1 R) \\ \frac{j\omega\varepsilon_m}{\gamma_1} I'_m(\gamma_1 R) - \sigma_g I_m(\gamma_1 R) & -\frac{m\beta}{\gamma_1^2 R} I_m(\gamma_1 R) & -\frac{j\omega\varepsilon_d}{\gamma_2} K'_m(\gamma_2 R) & \frac{m\beta}{\gamma_2^2 R} K_m(\gamma_2 R) \\ \sigma_g \frac{m\beta}{-\gamma_1^2 R} I_m(\gamma_1 R) & I_m(\gamma_1 R) - \sigma_g \frac{j\omega\mu_m}{\gamma_1} I'_m(\gamma_1 R) & 0 & -K_m(\gamma_2 R) \end{vmatrix} = 0 \quad ..(14)$$

By analytically solving the above equation, dispersion relation for fundamental mode (m=0) can be computed as:

$$\frac{\varepsilon_d K'_0(\gamma_2 R)}{k_2 K_0(\gamma_2 R)} - \frac{\varepsilon_m I'_0(\gamma_1 R)}{k_1 I_0(\gamma_1 R)} = \frac{j\sigma_g}{\omega}$$

where:

$K'_0(\gamma_2 R)=-K_1(\gamma_2 R)$ and $I'_0(\gamma_1 R)=I_1(\gamma_1 R)$ (Saeed *et al.*, 2020). For the detailed understanding of propagating surface wave, influence of different parameters such as chemical potential of graphene, thickness of waveguide and refractive index of outer environment on its propagation, the numerical results are computed and presented in the next section.

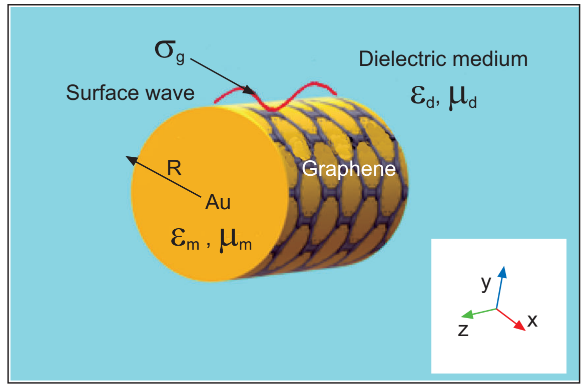

Fig. 1. Metal graphene dielectric based cylindrical structure.

Results and Discussion

The numerical analysis of the proposed structure is performed using the Wolfram Mathematica software package student version. The characteristics of fundamental transverse magnetic (TM) SPP mode along the MGD interface are computed. The environment is considered as isotropic dielectric with permitivity $3\varepsilon_O$ and permeability μ_o. The relaxation time is taken as 1.66 ps alongwith *T*=300 K. The chemical potential of the graphene was kept as 0.5 eV. The spatial dependence alongwith the field profile of the guided modes demonstrates the difference between surface plasmon modes and waveguide modes. Surface plasmon modes are excited on the interface of two media. These modes die down exponentially while travelling away from the interface (Yaqoob *et al.*, 2018). The excitation and propagation of the surface waves is evident from the Fig. 2 as depicted by the field profile of the fundamental mode as a function of radius for MGD. The field profile is generated on the basis of field equation no. 8, provided in previous section.

A comparison of the dispersion curve of graphene coated metallic cylindrical waveguide embedded in dielectric environment and the dispersion curve for the surface waves at the dielectric graphene and dielectric nanowire as the function of the THz frequency is presented to confirm the convergence of the analytical methodology and numerical modelling proposed in the present study (Gao *et al.*, 2014) with *T*=300 K, τ=1.66 ps and μ_c=0.5 eV keeping the permittivity of the environment as ε_o. The results of the present work exhibited a good agreement with published literature as shown in Fig. 3. The use of graphene coated metal also appeared to be advantageous

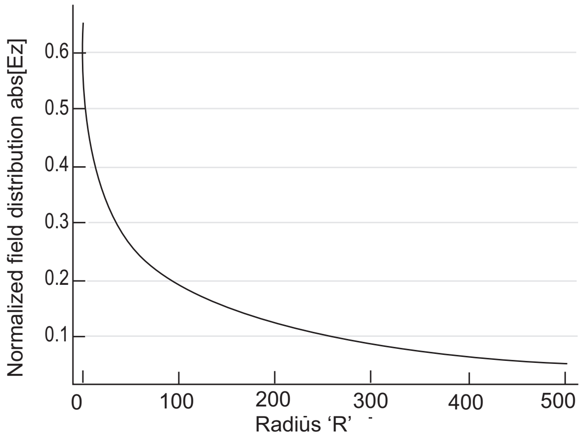

Fig. 2. Normalized field distribution for metal-graphene dielectric circular waveguide as function of radius with T=300 K, τ=1.66 ps and μ_c=0.5 eV.

in terms of providing higher values of propagation constant representing better field confinement.

Figure 3 defines comparison of dispersion curve of graphene plasmon fundamental mode in published literature (Gao *et al.*, 2014) and dispersion curve of graphene plasmon fundamental mode in present work with special conditions.

Keeping in view the tight field confinement supported by nobel metals such as gold, silver etc. gold is assumed as supporting metal with plasmon frequency ω_p=1.30 × 10^{16} rad/s and damping factor γ=2.80×10^{13} rad/s as indicated by the Drude Model (Yaqoob *et al.*, 2018). The frequency (ω) is normalized by the surface plasmon resonance frequency $\omega_{sp}=\omega_p/\sqrt{1+n_c^2}$ and the propagation constant (β) is normalized by $K_{sp}=\omega_{sp}/c$. The dispersion curve is plotted between the normalized frequency (ω/ω_{sp}) and the normalized propagation constant (β/k_{sp}) in Fig. 4 to examine the propagation of surface waves along MGD interface which represents a forward propagating surface wave with strong field confinement alongwith the cut off normalized frequency of 0.5.

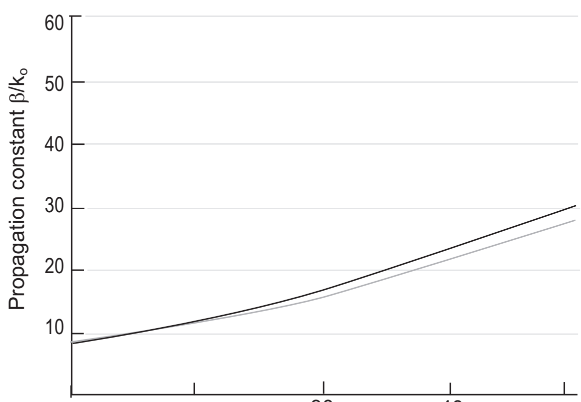

Fig. 3. Comparison of dispersion curves of the fundamental mode of graphene SPPs in published literature (Vakil and Engheta, 2011) and present work under special conditions.

Figure 4 describes dispersion relation for the graphene coated metallic cylindrical waveguide in dielectric medium with μ_c=0.5 eV, T=300 K and τ=1.66 ps. The chemical potential of graphene $\mu_c = h v_f \sqrt{n_c \pi}$ plays an important role for the active manipulation of the surface waves. The chemical potential depends upon the carrier concentration and gating voltage, as described in (Efetov and Kim, 2010). The propagation behaviour of surface waves is demonstrated by generating simulations for normalized propagation constant and normalized frequency as a function of chemical potential ranging from 0.2 eV to 1.5 eV (e.g., μ_c=0.2 eV, μ_c=0.7 eV, μ_c=1.2 eV, μ_c=1.5 eV).

Figure 5 displays that confinement of surface waves significantly reduces with rise in chemical potential. The slow moving surface waves exhibit cutoff free propagation for smaller values of chemical potential. However the reduction in propagation constant indicates

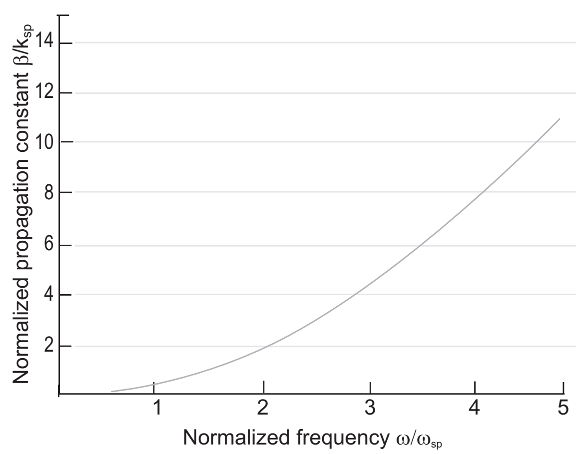

Fig. 4. Dispersion relation for the graphene coated metallic cylindrical waveguide in dielectric medium with μ_c=0.5 eV, T=300 K and τ=1.66 ps.

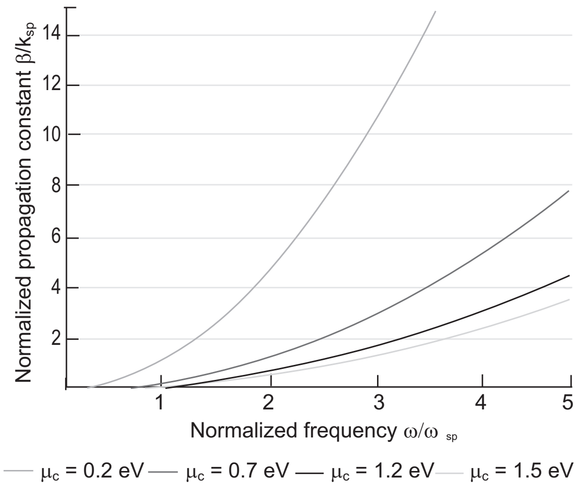

Fig. 5. Influence of chemical potential with T=300 K, τ=1.66 ps and R=100 nm on dispersion curve of MGD.

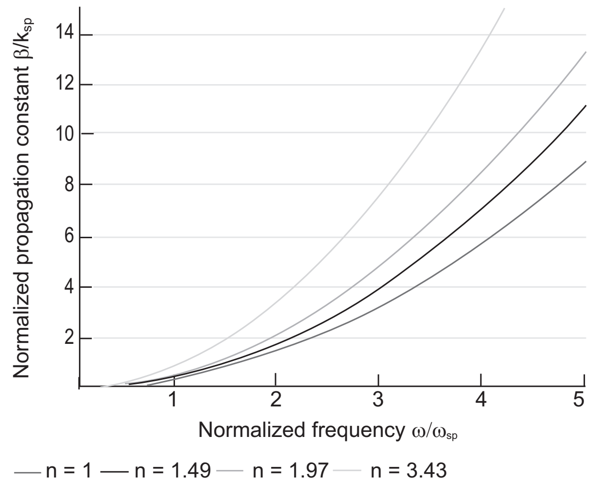

Fig. 6. Influence of refractive index of environment on dispersion curve of MGD with T=300 K, τ=1.66 ps, and μ_c=0.5 eV.

the presence of fast moving less localized surface waves (Saeed *et al.*, 2020).

Higher values of permittivity of the surrounding dielectric tend to confine the surface waves near the interface between the metal and dielectric, as depicted by (He *et al.*, 2013; Gan *et al.*, 2012). Therefore, the nature of the surrounding dielectric material significantly alter the propagative behaviour of surface waves. The refractive indices of dielectric are assumed as (n=1, n=1.49, n=1.97 and n=3.43) representing air, silica, silicon carbide and silicon keeping in view the natural abundance and physical access of these materials for the realization of the proposed structure. The permeability of both metal and dielectric is considered to be constant (i.e., $+1\mu_0$). The dispersion curve presented in Fig. 6 illustrates that strongly confined plasmon modes propagate when waveguide is embedded in silicon environment. However, the confinement of surface waves is significantly damped when air is used as surrounding environment. These results show a good agreement with (Gan *et al.*, 2012).

Surface waves exhibit a special kind of propagation behavior. i.e., these waves move along the interface and die down when move away from interface. So, geometrical parameters such as radius of the cylindrical waveguide is a crucial parameter for the modulation and manipulation of the surface waves. Figure 7, depicts the confinement of the surface modes as a function of radius of the cylindrical waveguide. The dispersion

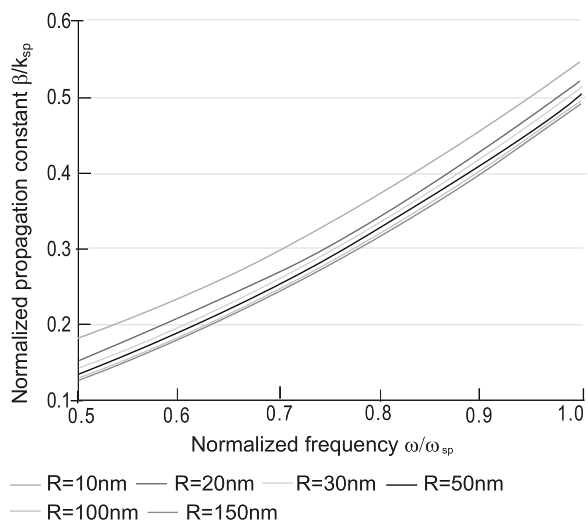

Fig. 7. Influence of radius with T=300 K, τ=1.66 ps, and μ_c=0.5 eV for graphene coated metallic cylindrical waveguide.

curve is plotted for various values of radius i.e., 10 nm, 20 nm, 30 nm, 50 nm, 100 nm and 150 nm. Strongly confined cutoff free surface modes are noticed for the cylindrical waveguide of the order of 20 nm (Achanta, 2020). A significant reduction in localization of these modes occurs with an increase in radius which is due to the decay of surface waves away from the interface. The further increase in radius greater than 100 nm displayed persistent behaviour of propagation constant as indicated by the overlapping of the dispersive curves, while the coupling between the plasmon modes at the metal dielectric interface gets stronger as the metal thickness is less than 50 nm (Achanta, 2020).

Conclusion

Theoretical and numerical investigations are presented to study the characteristics of the surface wave propagating along the interface of a monolayer graphene coated metallic cylindrical waveguide embedded in a dielectric environment. The surface waves are found to be sensitive to graphene parameters and nature of the materials acting as environment. The dispersion relation is computed for the proposed geometry and the following conclusions are drawn:

- The field distribution for the MGD cylindrical structure represents the existence of surface waves.
- The surface waves are found to be less localized for higher values of the chemical potential of graphene.
- The radius of the cylinder is a crucial parameter in order to tune and manipulate the propagation characteristics of the surface waves as confinement of surface waves is found sensitive to the radius of the waveguide.
- The confinement of the surface waves is found to be sensitive to the refractive index of the surrounding environment of the cylinder. The use of high indexed material as an environment may lead to strongly confined plasmon modes.
- The proposed structure due to the dynamic controllability of surface waves, may have potential applications in wave propagation, modulators, spectroscopy, circular polarizers, nanoscale interconnects for optical circuits and switching.

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Conflict of Interest. The authors declare that they have no conflict of interest.

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