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Theoretical Study of Surface Waves in Hexagonal Boron Nitride (hBN)

REVIEW ARTICLE

Arjun Mishra[1*]
Research Scholar,
Department of Physics, University of Lucknow, Lucknow, UP, India.
misharju25@gmail.com

Daya Shanker
Associate Professor
Department of Physics, University of Lucknow, Lucknow, UP, India.

Utkarsh Kumar Sharma
Research Scholar
Mechanical Engineering, KNIT, Sultanpur, UP, India

Amit Medhavi
Research Scholar
Mechanical Engineering, KNIT, Sultanpur, UP, India

Abstract

Hexagonal boron nitride (hBN) is a wide bandgap semiconductor material in which Boron (B) and Nitrogen (N) atoms form hexagonal structure and has number of robust properties of technological importance. Boron nitride nanotubes (BNNTs) are very nice area of research in recent years. Its structure is similar to carbon nanotubes (CNTs) where carbon atoms are arranged in hexagon. hBN is also known as White Graphene. Various methods are employed to synthesize hBN such as laser ablation method, arc-discharge method, chemical vapor deposition method, ball-milling method, and thermal plasma arc method etc. When electromagnetic (EM) wave falls on the semiconductor surface, some waves can be excited such as Plasmons (quanta of valence electron oscillation), Phonons (quanta of lattice vibration) and Excitons (quanta of electron-hole pair oscillation). When photon (quanta of em wave) of the incident em wave is coupled with these excitations, coupled modes can be generated. These modes are called polariton modes. In this paper, planar interface between semi-conductor hexagonal Boron Nitride (hBN) and vacuum is taken for the study of coupled surface oscillations. hBN also shows hyperbolic phonon polaritons (HPPs). To study the surface oscillations or waves, a dispersion relation is obtained from Maxwell equations, which gives frequency dependent dielectric function $\varepsilon(\omega)$ that must be negative for the existence of these waves. Two coupling frequency modes $\left(\frac{\omega}{\omega_p}\right)_+$ and $\left(\frac{\omega}{\omega_p}\right)_-$ are obtained. The first mode $\left(\frac{\omega}{\omega_p}\right)_+$ is obtained in ultraviolet (UV) region (10^{16}Hz) and the second mode $\left(\frac{\omega}{\omega_p}\right)_-$ is obtained in the Infrared (IR) region (10^{13} Hz). The surface wave exists when $\left(\frac{\omega}{\omega_p}\right)_+ < 0.47$ as for this range the dielectric function remains negative. The other $\left(\frac{\omega}{\omega_p}\right)_-$ mode remains nearly constant with values 0.006. hBN and BNNTs have also such nice properties, which are useful in various fields such as nano photonics, opto electronics, sensing, spectroscopy, thermal management techniques, energy storage etc. Various heterostructures of hBN with other materials like graphene, Silicon oxide (SiO_2), Silicon (Si) etc are useful in numerous fields. Waveguides, made up of hBN are very good for propagation of radiations in various spectral ranges.

Keywords: Dispersion relation, Dielectric function, Surface plasmon, Surface phonons, Polaritons.

INTRODUCTION

The polar semiconductor hexagonal boron nitride (hBN) has hexagonal structure and shown nice properties. Surface plasmons are the valence electron oscillations exist at the interface between semiconductor material and surrounding dielectric medium. The charge density of polar semiconductors is very high similar to a metal. When an electromagnetic (em) wave is incident on semiconductor surface, it transfers energy to the valence electrons hence polarization is induced and these valence electrons oscillate collectively with positive ions in the background and Coulomb force is acting between them. This is called plasma oscillation with plasmon as a quantum. These plasmons are transverse magnetic (TM) in nature. Bulk plasmons are also existed in the whole volume. Optical phonon modes also excited due to lattice vibration when em wave is incident. They are of two types: transverse and longitudinal [1]. If wave vector of incident photon match with the wave vector of plasma oscillation, surface plasmon resonance (SPR) is also observed. Earlier studies shown that doping enhances the SPR [2]. For surface plasmons existence, the frequency dependent dielectric function $\varepsilon(\omega)$ should be negative [3]. The existence of surface wave depends upon the material properties and frequency of incident wave. Various types of surface waves such as phonon polariton, exciton polariton, plasmon polariton and others can be excited and analyse by different methods [4]. Therefore the analysis of plasmon behavior in different materials has wide scope of research. Many theoretical and experimental studies showed the existence of surface plasmons in different important frequency ranges for different type of materials [5,6]. To study these excitations, various methods and techniques are there such as dispersion relation. The study of these surface plasmons and other surface excitation can be done theoretically with its help.

A number of models are there such as Bloch hydrodynamic model, Drude model, Lorentz model, combined Drude-Lorentz model etc to get this dispersion relation [7,8]. The interaction between various surface excitations such as phonon-plasmon interaction is also studied for various geometries of material e.g. planar, cylindrical and spherical etc with the help of these models [9-11]. The properties of these oscillations can be varied on varying the conditions of surroundings [12]. Research and analysis of different materials is continuously growing at present as these waves have tremendous properties and they have great role in various technologies [13-18]. Carbon Nanotubes (CNTs) have shown many types of surface excitations [19-26], which are useful in sensing techniques [27], lithography [28] and others. They also play a nice role in the enhancement of different kinds of Raman scattering techniques [29-33]. Nanotubes of hBN also have shown very robust properties [34]. Here we have investigated the conditions; for which the coupled plasmon-phonon waves exist at the plane surface of hexagonal Boron-Nitride (hBN) semiconductor.

hBN, a 2D material have great applications in number of areas. It is also known as white graphene. It has same hexagonal structure as graphene. The hyperbolic phonon polaritons (HPPs) shown by the hBN have nice role in nano-antenna, hyper lensing etc. the HPPs of hBN can couple with the surface plasmon polaritons (SPPs) of monolayer graphene to generate hybrid mode. At room temperature, hBN shown luminescence in range 215-227 nm. It also shows strong coupling between excitons and phonons. In single photon emission (SPEs), hBN have great place. A thin layer of hBN between two parallel layers of conducting transition metal di-chalcogenides (TMDs) support dissipation-less exciton super fludity and it has great role in energy efficient technologies. Due to high thermal conductivity, electrical insulation and chemical stability, hBN also used in thermal management of devices [35].

hBN is synthesized in labs by various methods, which are arc-discharge method, laser-ablation method, chemical vapor deposition (CVD) method, ball milling method, thermal plasma jet method etc. hBN nanotubes are employed in advance nanomaterials for mechanical strength, neutron shielding in space to protect space devices etc. In arc-discharge method, anode and cathode are present and plasma arc vaporizes the anode part, containing compound of boron and nitrogen. Single-walled and multi-walled BNNTs are formed but low yield of nanotubes is a disadvantage of this method. CNTs, which are almost similar to BNNTs in structure are largely produced by chemical vapor deposition (CVD) method. BNNTs are also produced by this method. By Laser Ablation method, high quality single-walled and multi-walled BNNTs can be synthesized. Thermal Plasma Jet method is employed for high yield BNNTs and Ball Milling method is useful in production of BNNTs at low cost in industries [36].

Good quality monolayer of hBN is very promising in 2D heterostructures [37]. Waveguides made up of multilayer graphene and hBN supports mid-infrared signals and they are useful in various fields [38]. Two dimensional (2D) hBN is useful in electrochemistry as electro-analytical sensing tool[39]. High quality nano-ribbons of graphene can be grown in hBN stacks for high performing electronic devices [40]. The spin defects in solid state materials such as hBN are employed in quantum sensors[41]. hBN has a wide bandgap of nearly 5.96 eV but it shows luminescence in deep ultra-violet region due to strong electron-phonon interactions [42]. hBN/graphene stacked van der Waals heterostructures can be grown on copper foils and they are useful in energy band modulation [43]. hBN based heterostructures are highly promising for future applications, one of this is obtained by transferring sheet of hBN crystal on to SiO_2/Si substrate and reduced graphene oxide substrate[44]. Using hBN addition, the dielectric properties of Zinc Oxide (ZnO) nanoparticles is improved and such nanocomposite materials have great applications [45]. In hBN-graphene metamaterials, surface plasmon-phonon polaritons are obtained [46].

METHODOLOGY

The frequency dependent dielectric function $\varepsilon(\omega)$ must be negative for the existance of the surface waves so it is necessary to analyse the nature of $\varepsilon(\omega)$. The frequency dependent dielectric function is given by the following equation to study the coupled surface plasmons-phonon wave on the planar surface of these polar semiconductors (here hBN is taken as semi-conductor) surrounded with vacuum [47]:

$$\varepsilon(\omega) = \varepsilon_L(\omega) - \frac{\omega_p^2}{\omega^2} \tag{1}$$

$$\varepsilon(\omega) = \frac{\varepsilon_\infty \omega^2 - \varepsilon_0 \omega_t^2}{\omega^2 - \omega_t^2} - \frac{\omega_p^2}{\omega^2} \tag{2}$$

Where $\varepsilon_L(\omega) = \frac{\varepsilon_\infty \omega^2 - \varepsilon_0 \omega_t^2}{\omega^2 - \omega_t^2}$ (3)

is the lattice dielectric function.

$\omega_p = PlasmaFrequency$

ω_t = Transverse optical phonon frequency

ε_o = Static dielectric constant of semiconductor

ε_∞ = Optical dielectric constant

$$\frac{\omega_p^2}{\omega^2} = \frac{\varepsilon_\infty \omega^2 - \varepsilon_0 \omega_t^2}{\omega^2 - \omega_t^2} - \varepsilon(\omega) \tag{4}$$

$$\frac{\omega^2}{\omega_p^2} = \frac{1}{\frac{\varepsilon_\infty \omega^2 - \varepsilon_0 \omega_t^2}{\omega^2 - \omega_t^2} - \varepsilon(\omega)} \tag{5}$$

$$\frac{\omega^2}{\omega_p^2} = \frac{1}{\frac{\varepsilon_\infty \frac{\omega^2}{\omega_p^2} - \varepsilon_o \frac{\omega_t^2}{\omega_p^2}}{\frac{\omega^2}{\omega_p^2} - \frac{\omega_t^2}{\omega_p^2}} - \varepsilon(\omega)} \tag{6}$$

The above equation (6) is reduced to the following form

$$\left(\frac{\omega}{\omega_p}\right)^4 \{\varepsilon_\infty - \varepsilon(\omega)\} + \left(\frac{\omega}{\omega_p}\right)^2 \left\{\varepsilon(\omega)\left(\frac{\omega_t}{\omega_p}\right)^2 - \varepsilon_o\left(\frac{\omega_t}{\omega_p}\right)^2 - 1\right\} + \left(\frac{\omega_t}{\omega_p}\right)^2 = 0 \tag{7}$$

The equation (7) is quadratic in$\left(\frac{\omega}{\omega_p}\right)^2$ and roots of this equation can be found with the help of quadratic formula. On varying the value of dielectric function $\varepsilon(\omega)$, different roots can also be found. On solving above equation, we get$\left(\frac{\omega}{\omega_p}\right)^2$. From $\left(\frac{\omega}{\omega_p}\right)^2$, $\left(\frac{\omega}{\omega_p}\right)_+$ and $\left(\frac{\omega}{\omega_p}\right)_-$ are calculated. The graph between dielectric function $\varepsilon(\omega)$ and $\left(\frac{\omega}{\omega_p}\right)$ is plotted with variation in the values of $\varepsilon(\omega)$ with the help of MS Office Excel software. This graph is analyzed and the condition for the appearance of surface wave is obtained for the planar surface of hBN.

RESULTS AND DISCUSSION

For obtaining the coupled surface plasmon-phonon modes, value the frequency dependent dielectric function $\varepsilon(\omega)$ is varied and the roots $\left(\frac{\omega}{\omega_p}\right)_+$ and$\left(\frac{\omega}{\omega_p}\right)_-$ are obtained. The values of various parameters $\omega_p, \omega_t, \varepsilon_0 \wedge \varepsilon_\infty$ are obtained from well established earlier studies [47, 48].

hBN

ω_p = 3.74530120 X 10^{16} Hz, ω_t = 25.64963855 X 10^{13} Hz, ε_o= 6.8, ε_∞= 4.46

Table 1: Variation in frequency modes $\left(\frac{\omega}{\omega_p}\right)_+$ and $\left(\frac{\omega}{\omega_p}\right)_-$ with dielectric function $\varepsilon(\omega)$ for hBN

S.No.	$\varepsilon(\omega)$	$\left(\frac{\omega}{\omega_p}\right)_+$	$\left(\frac{\omega}{\omega_p}\right)_-$
1	-1	0.427983982	0.0068
2	-0.5	0.449037899	0.0068
3	0	0.473539712	0.0068
4	0.5	0.502546487	0.0068
5	1	0.537625780	0.0068

Here in Table 1 the value of dielectric function $\varepsilon(\omega)$ is varied from -1 to 1 therefore the value of frequency mode $\left(\frac{\omega}{\omega_p}\right)_+$ increases from nearly 0.42 to 0.53 but the other frequency mode $\left(\frac{\omega}{\omega_p}\right)_-$ remain constant nearly at value 0.0068.

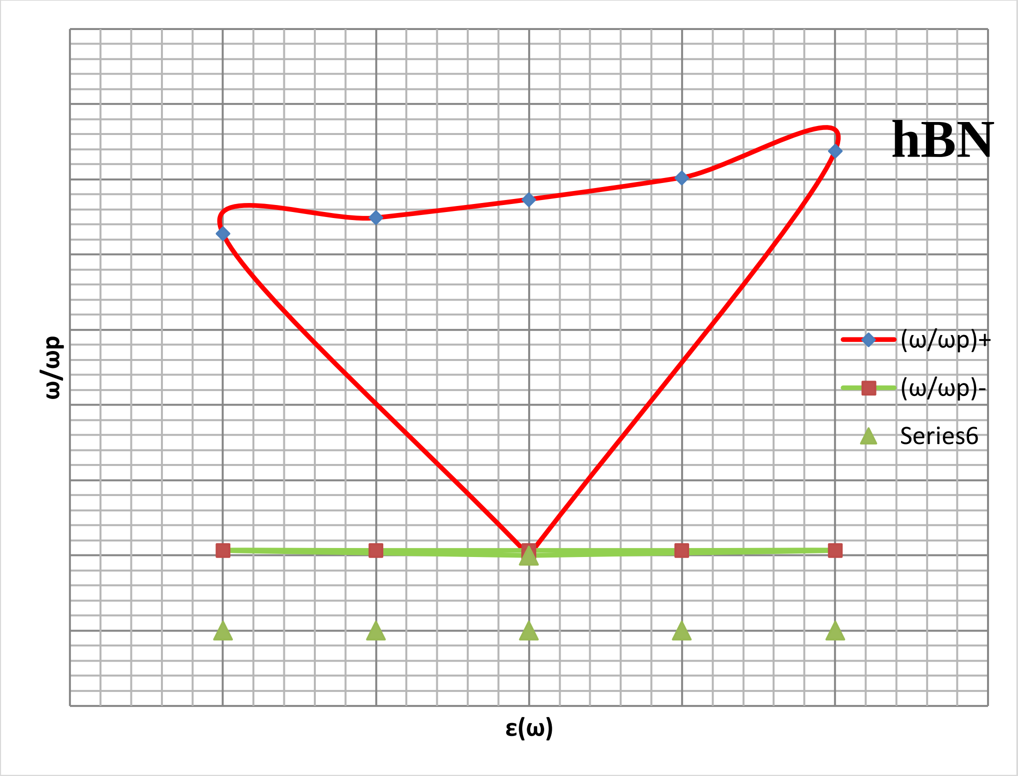

Figure 1: Graph showing variation of $\frac{\omega}{\omega_p}$ with $\varepsilon(\omega)$ for hBN (Red line curve represents $\left(\frac{\omega}{\omega_p}\right)_+$ and light green line curve represents $\left(\frac{\omega}{\omega_p}\right)_-$)

From the above graph in Figure 1 between $\frac{\omega}{\omega_p}$ and $\varepsilon(\omega)$ for hBN, we analyse the behavior of $\left(\frac{\omega}{\omega_p}\right)_+$ and $\left(\frac{\omega}{\omega_p}\right)_-$. The $\left(\frac{\omega}{\omega_p}\right)_+$ line is represented by red line and $\left(\frac{\omega}{\omega_p}\right)_-$ line is represented by light green line. $\varepsilon(\omega)$ is negative when $\left(\frac{\omega}{\omega_p}\right)_+$ is less than or equal to 0.47. Hence in this range, surface waves exist.

If $\left(\frac{\omega}{\omega_p}\right)_+$ is greater than the above obtained range then $\varepsilon(\omega)$ becomes positive and surface wave not obtained because it is transmitted after passing through the material. The highly localized surface excitations are obtained when its frequency lie close to that of the surface plasmons. The modes in different frequency region have their specific importance in number of fields. The plasmon frequency is of the order of 10^{16} Hz in this case and it lies in ultraviolet (UV) range, so the coupled modes $\left(\frac{\omega}{\omega_p}\right)_+$ are obtained in UV region. The second frequency mode $\left(\frac{\omega}{\omega_p}\right)_-$ remains nearly constant throughout for all values of $\varepsilon(\omega)$ taken here. For hBN, it is nearly equal to 0.0068. The $\left(\frac{\omega}{\omega_p}\right)_-$ modes are in infrared (IR) range (10^{13} Hz).

There are various other tremendous properties of hBN, which are yet to be investigated. From the above properties and applications of hBN and BNNTs, it is clear that more research studies are required on it and other such materials.

CONCLUSION

hBN nanotubes have nice properties useful in new technologies. They are produced by different methods for different purposes, some for high yield and some for good quality. It is seen that using dispersion relation, study the surface waves on BNNTs can be done theoretically. Two coupled surface plasmon-phonon modes one is obtained in the UV region and other in IR region. The surface waves on a material in different frequency ranges have great role in the modern technologies. Such type of studies on other materials with different geometries (planar, spherical, cylindrical etc) led to the large scale advancements. BNNTs have shown great role in nanotechnology, opto-electronics, waveguides, sensing, space research, energy storage and other fields.

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