Theoretical Investigation of Phonon – Polariton Modes in Cylindrical Hexagonal Boron Nitride

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What is Phonon – Polariton?

- Phonon-polariton is a quantum mechanical phenomena where it can be considered a boson(quasi)-particle that is resulted from the strong coupling of infrared photon and optical phonon.
- These coupling occurs at the region where the energies of phonon and polariton overlap one another, henceforth creating a so-called quantum mechanical (quasi-) particle which possess the properties of both photon and phonon. Figure 1 shows the dispersion relation curve of coupled phonon-polariton.

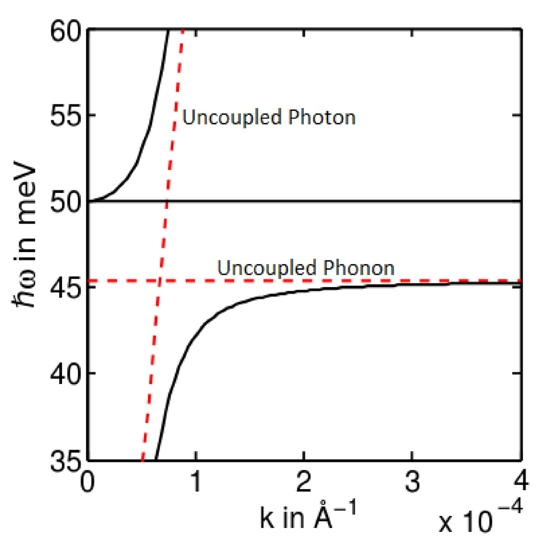

Figure 1. A generic coupled phonon-polariton dispersion relation (black lines). The red dash lines represent the dispersion relation of uncoupled photon and phonon particles.

Phonon-Polariton in Hyperbolic Material

- A hyperbolic material is characterized by an anisotropic permittivity (or permeability) tensor, where the principle components of in-plane (for example x- and y- axis in figure 2) have different sign than the principle component of out-of-plane (z- axis in figure 2).
- When the coupling of phonon-polariton occurred in this type of material, a special kind of optical mode called hyperbolic phonon-polariton (HP) can be induced. These modes allows extreme confinement of HP in the sub-diffractional scale and propagation within the hyperbolic material with essentially low losses.
- Based on these hyperbolic properties we can then classify it into type I and type II, where type I (figure 3b) holds the permittivity $\varepsilon_x,\varepsilon_y > 0,\ \varepsilon_z < 0$, and type II (figure 3c) have the permittivity opposite sign of type I, that is, $\varepsilon_x,\varepsilon_y < 0,\ \varepsilon_z > 0$.

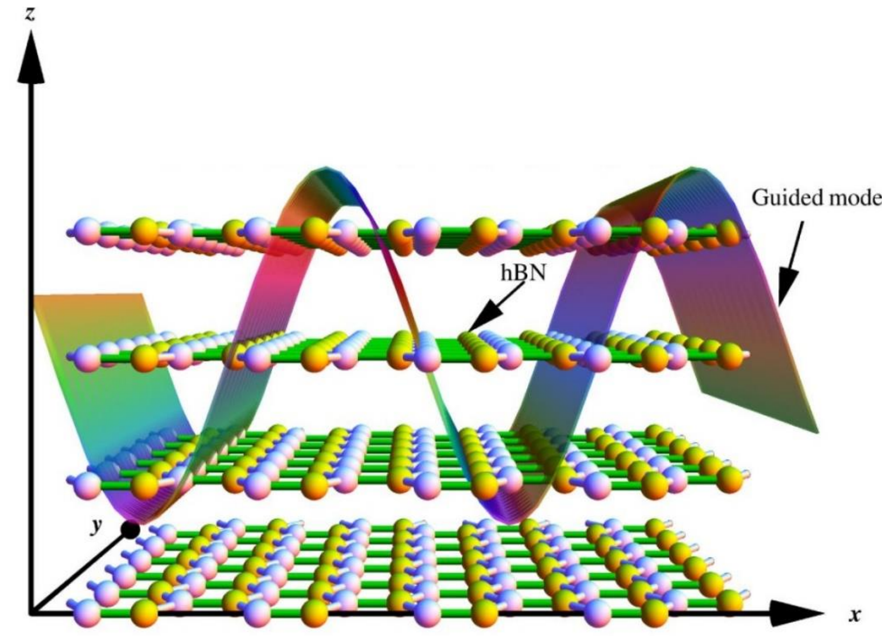

Figure 2. A schematic of guided wave in hexagonal boron nitride (hBN) structure. Figure adapted with permission from Ref. 1.

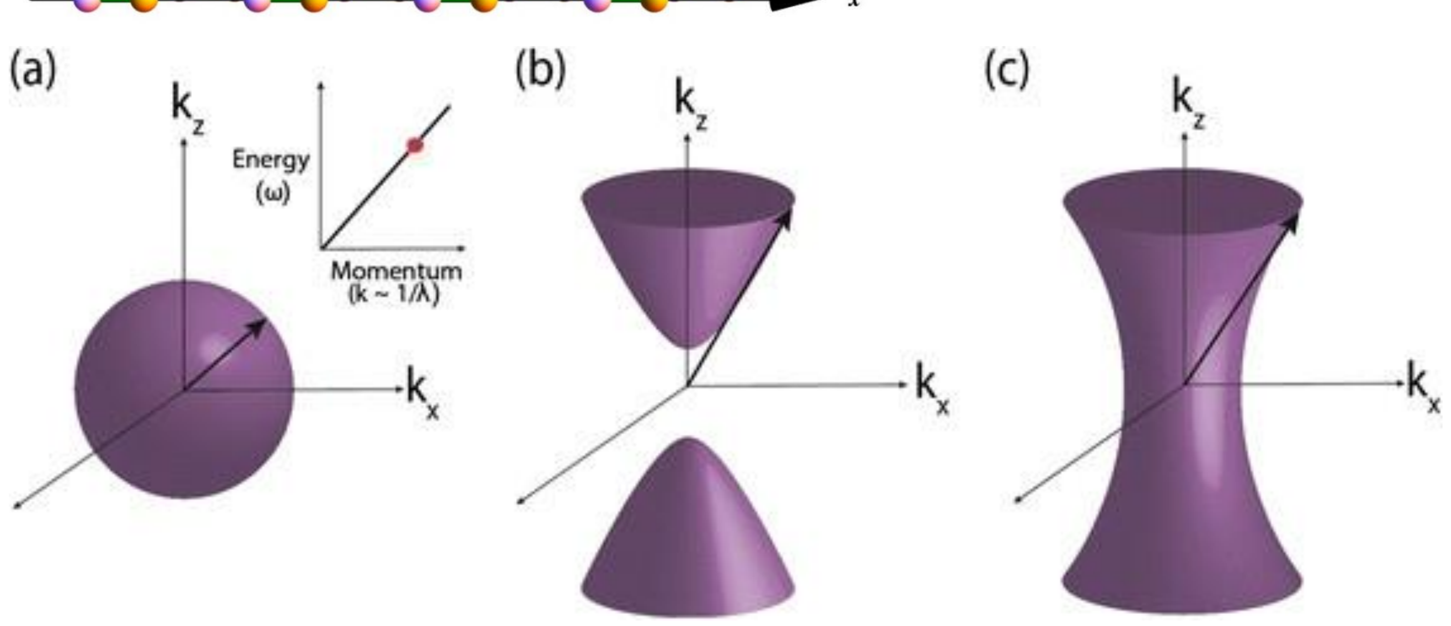

Figure 3. Schematic k-space for different types of material. (a) The spherical isofrequency surface is an indication of an isotropic material with all ε_x, ε_y, ε_z having the same sign. The hyperboloid isofrequency surface of (b) type I and (c) type II material on the other hand, holds the permittivity (b) $\varepsilon_x,\varepsilon_y > 0,\ \varepsilon_z < 0$ and (c) $\varepsilon_x,\varepsilon_y < 0,\ \varepsilon_z > 0$ respectively. Figure taken from Ref. 2 under Creative Common License.

Abstract

Hexagonal boron nitride (hBN) is a two-dimensional material which can be found in nature. With several layers stacked on top each other, hBN is able to exhibit opposite sign of in-plane (defined perpendicular notation ⊥) and out-of-plane (defined parallel notation ∥) components. This exotic property, along with the phonon-polariton coupling forms the hyperbolic dispersion and high wave-vector confinement modes in the type I and type II regions, also known as Reststrahlen bands. Here we report on three-dimensionally confined hyperbolic phonon-polariton (HP) in cylindrical hexagonal boron nitride that supports (theoretically) infinite orders of HP modes in the Reststrahlen bands. Moreover, we found the symmetry of cylindrical structure in nature allows for infinite sets of those orders.

Method

- To understand the phonon-polariton coupling modes in hBN, we first solve Maxwell equation in the cylindrical coordinate and assume ansatz electric field, $\vec{E} = \vec{R}_1(r)e^{-in\phi}e^{-ik_z z}e^{-i\omega t}$ and magnetic field, $\vec{B} = \vec{R}_2(r)e^{-in\phi}e^{-ik_z z}e^{-i\omega t}$. Moreover, from ref. 2, we consider the hBN permittivity to be:

$$\epsilon_m(\omega) = \epsilon_{\infty,m} + \epsilon_{\infty,m} \times \frac{(\omega_{LO,m})^2 - (\omega_{TO,m})^2}{(\omega_{TO,m})^2 - \omega^2 - i\omega\Gamma_m}$$

- Where m = ⊥, ∥. Here $\epsilon_{\infty,m}$ is the electronic contribution to the permittivity, Γ_m is the damping coefficients from the phonon contribution, and $\omega_{LO,m}$ and $\omega_{TO,m}$ are the longitudinal and transverse frequency which we have described above.
- The obtained Maxwell solution is then apply to air-hBN-air boundary conditions (see figure 4) to compute its determinant.
- For simulation purposes, we utilized MATLAB and COMSOL MULTIPHYSICS commercial software package to determine the dispersion relation of cylindrical hBN.

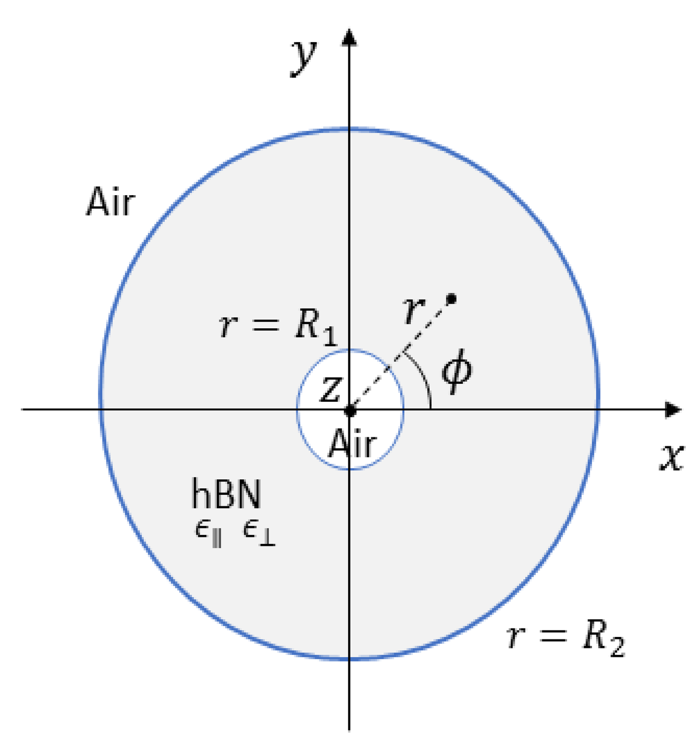

Figure 4. A schematic structure of hBN in cylindrical coordinate, represented by r,φ,z (coming out of the page) components. Two permittivity components $\epsilon_\parallel$ and $\epsilon_\perp$ are denotes as out-of-plane and in-plane in the hBN medium, respectively.

Conclusion

- In summary, the project consists in finding the theory and simulation of sub-diffractional guided wave confined in cylindrical hexagon boron nitride.
- We solve Maxwell equation in cylindrical coordinate and apply air-hBN-air boundary conditions (see figure 4) to compute its determinant.
- The results presented here demonstrate the dispersion relation of type II Reststrahlen band, where the band frequencies ranges from $\omega_{TO,\perp} = 1370\ cm^{-1}$ to $\omega_{LO,\perp} = 1610\ cm^{-1}$.
- We obtain an infinite sets of hyperbolic phonon-polariton (HP) modes for each $n = 0, 1, 2, \ldots$ up to infinity, where the angular parameter n is due to the symmetry of cylindrical structure in nature. In the previous experimental studies, so far only up to 7th order of HP modes [3] for $n = 0$ has been produced. However, other HP modes which constitutes $n > 0$ have not yet been observed.

Result

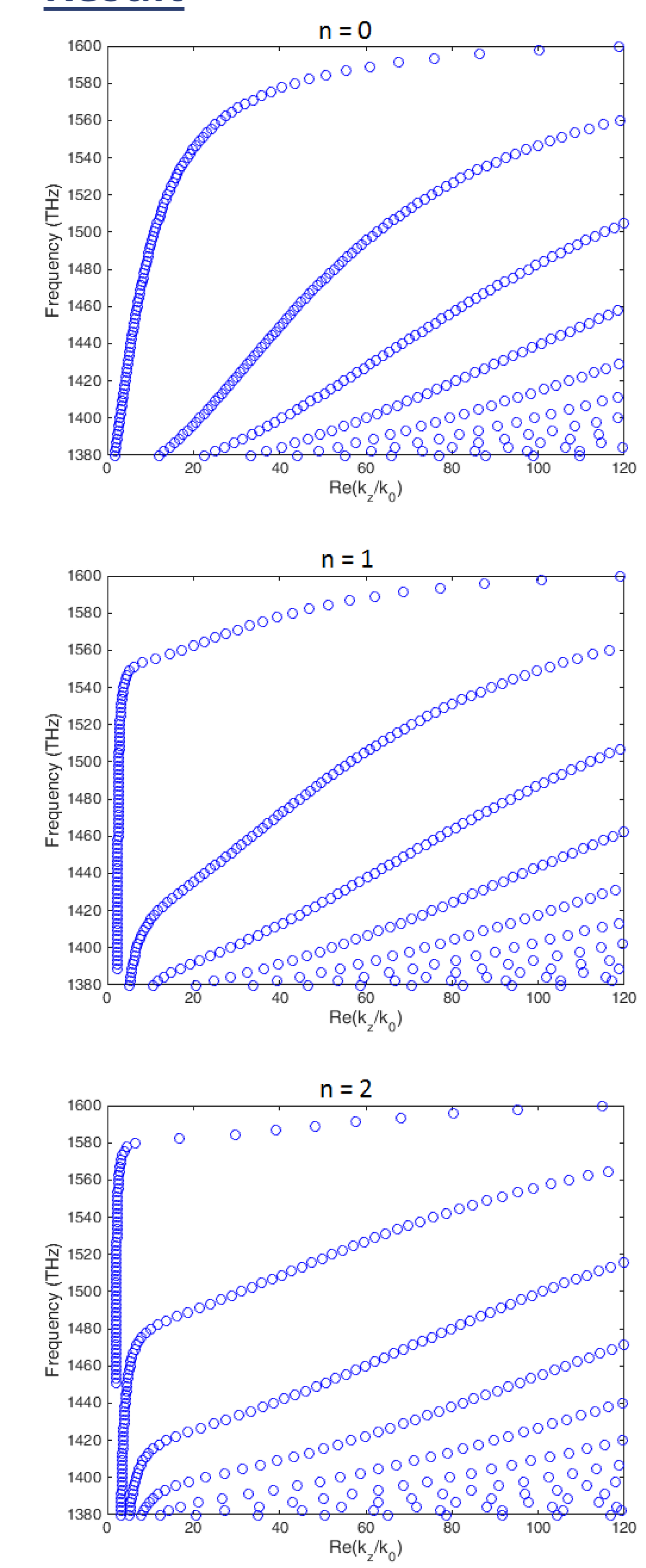

Figure 5. Dispersion relation curves of type II Reststrahlen band in cylindrical hBN. Each plot contain infinite order of HP modes (here we observe only up to 10 modes), and represent an angular dependent parameter $n = 0, 1, 2$. Note that the nature of the parameter n is an integer number from zero to infinity, and for our purposes we only performed the simulations up to $n = 2$.

Reference

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