

A Study on Light Coupling Effects in Hexagonal Boron Nitride Crystals for Quantum Photonic Designs

Yanan Wang* and Philip X.-L. Feng*

Electrical Engineering and Computer Science, Case School of Engineering, Case Western Reserve University, OH 44106, USA

**yanan.wang@case.edu; philip.feng@case.edu*

Abstract: We explore the light interaction effects in two-dimensional hexagonal boron nitride (h-BN) crystals and device structures at the wavelengths compatible with the defect-related quantum emission. The study paves the way to constructing integrated photonic circuitry based on this emerging quantum material. © 2019 The Author(s)

OCIS codes: (160.2220) Defect-center materials; (300.6280) Spectroscopy, fluorescence and luminescence; (130.3130) Integrated optics materials.

1. Introduction

Hexagonal boron nitride (h-BN), an attractive material that can enable atomically thin structures and - two-dimensional (2D) devices from its bulk crystals, possesses ultrawide electronic bandgap (5.9 eV) and excellent chemical and thermal stability [1]. Very thin h-BN crystals have primarily been employed as atomically smooth high- κ dielectric and encapsulation layers in 2D electronics and optoelectronics. The outstanding mechanical properties of h-BN (a Young's modulus theoretically predicted to be as high as $E_Y \sim 780$ GPa and a very high breaking strain limit of $\sim 22\%$) also enable h-BN 2D nanoelectromechanical systems [2,3]. Recently, h-BN has emerged as a promising platform for nanophotonics as well, hosting hyperbolic phonon-polaritons and robust quantum emitters at room temperature [4, 5]. However, a small refractive index of h-BN (~ 1.8) impedes the exploitation in the photonic domain, which makes it hard to achieve a high refractive index contrast that is required for efficient light confinement in the visible spectral range [6]. Also, due to the crystal anisotropy (in-plane vs out-of-plane), h-BN retains both ordinary and extraordinary indices. However, such birefringence effects have rarely been investigated on the device platform. With the aim to resolve these issues, we characterize the light-matter interaction in h-BN layers. Combining experimental measurements with numerical simulations, we have systematically evaluated the influence of crystal thickness, dielectric environment, excitation wavelength on the light out-coupling efficiency. We demonstrate that the light is engaged in multiple reflections with h-BN layers and underlying substrates, forming interferences that lead to enhancement or attenuation of the incoming and outgoing intensity of light. Moreover, mode analysis has been performed based on h-BN ridge waveguide taking consideration of the optical anisotropy. The present work provides valuable guidelines to design and optimize the photonic devices based on h-BN towards integrated photonic systems.

2. Experimental Results and Discussion

The h-BN samples are prepared via a suite of dry exfoliation and transfer techniques, as illustrated in our previous work [7]. h-BN flakes are mechanically isolated from a high-quality bulk h-BN crystal and pressed onto polydimethylsiloxane (PDMS) stamps. After exfoliation, the multilayer h-BN sheets with lateral size from tens to hundreds of micrometers are transferred onto patterned silicon dioxide on silicon (290-nm SiO_2/Si). As-prepared samples consist of supported and suspended h-BN regions (Figs. 1a & 1c), serving as ideal platforms to explore the influence of dielectric environment on the light coupling and optical contrast of h-BN. Prior to the optical characterization, high-temperature annealing at 850 °C under 1 Torr of nitrogen is performed to activate the defect centers and to desorb any possible surface contaminants.

Panels b & d of Fig. 1 present typical fluorescence microscopy images of h-BN devices, which are excited by a 532-nm laser through a high-magnification optical objectives (50 \times or 100 \times) and recorded by a highly sensitive spectrometry system (Princeton Instruments 2500). There are two types of emission can be observed in our h-BN devices. One exhibits broad emission across the entire visible spectrum, mainly from luminescent background (Fig. 1e). Another contains sharp peak features related to the quantum emission. As exemplified in Fig. 1f, the linewidth of these peaks can be as small as ~ 3 nm, which is closed to the lifetime-limited linewidth of h-BN quantum emitters at room temperature. Also, these narrow peaks are predominantly detected in proximity to 710 nm [8]. Therefore, the following discussion of optical contrast and waveguide mode analysis focus on this frequency range.

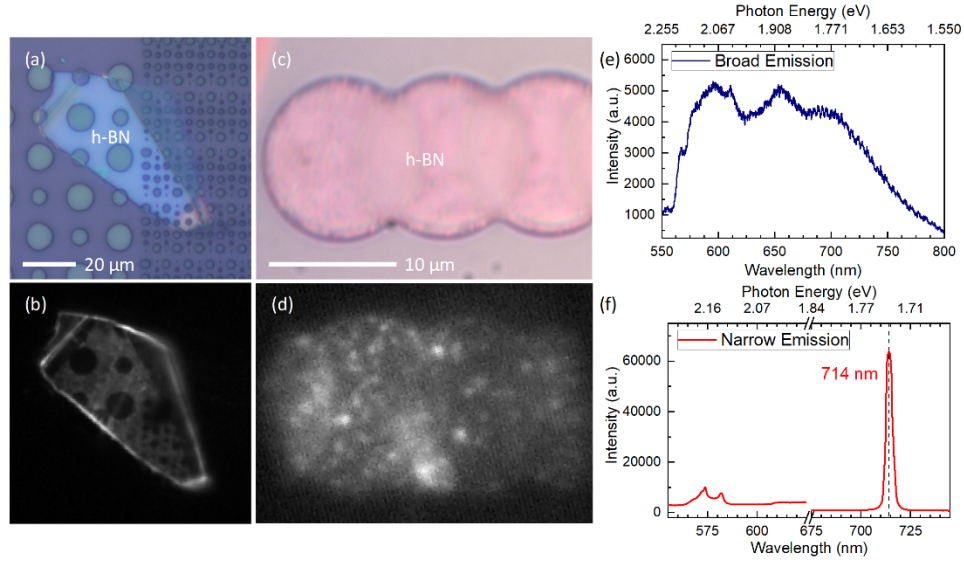


Fig. 1. (a)-(c) Optical and (b)-(d) fluorescence microscopy images of two h-BN samples on perforated SiO₂-on-Si substrate. (e)-(f) Typical emission spectra from h-BN samples with distinct profiles.

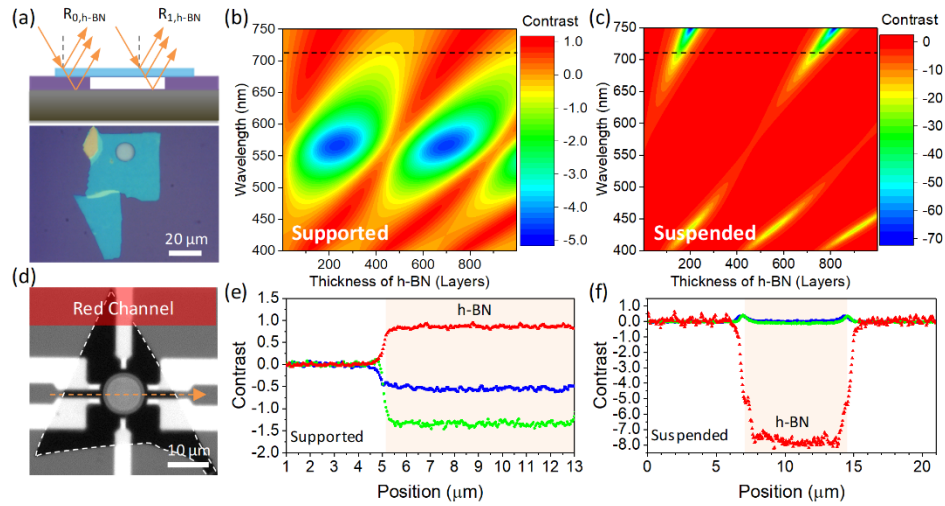


Fig. 2. (a) Schematic diagram of multi-reflection model and optical microscopy image for h-BN flake mechanically suspended over patterned SiO₂/Si. Color contour plots of the optical contrast as a function of h-BN thickness and excitation wavelength calculated by the Fresnel equations for (b) supported and (c) suspended cases. The wavelength of 710 nm is marked as black dash line. (d) Red-channel optical image of an h-BN nanoelectromechanical device and measured contrast traces of (e) supported areas and (f) suspended areas along the orange dashed line.

The optical contrast of h-BN is investigated based on the multi-reflection model illustrated in Fig. 2a and the Fresnel equations. The mechanically supported and suspended h-BN layers experience different dielectric environments and thereby exhibit distinct optical contrast. The optical contrast dependence on the h-BN thickness and the excitation wavelength is summarized in Fig. 2b & 2c. At the interested wavelength of 710 nm, the suspended case shows more prominent contrast value when the thickness of h-BN is around 200 nm (~ 600 layers). The difference in light outcoupling of supported and suspended devices can also be visualized in direct optical contrast measurement. For a 30-nm thick h-BN layer, the suspended region displays an optical contrast with opposite sign to the value from the supported area in the red-channel optical image with integrated gray value over 590 nm–720 nm (Fig. 2d).

The optical confinement of h-BN waveguide has also been studied by taking concern of the birefringence in the finite element method simulation (COMSOL Multiphysics). Fig. 3 shows the calculated effective indices for all the guided-modes supported in h-BN waveguide sitting on thick SiO₂ layer with fix width of 1 μ m and varied thickness from 350 nm to 1000 nm. Panels a & b of Fig. 3 are attained by assuming h-BN as a homogeneous medium with a normal refractive index of 1.8; while panels c & d are calculated based on setting the ordinary and extraordinary as

1.72 and 1.84, respectively. Typically, TE and TM modes propagate with different propagation constants and have different cut-off conditions. In order to support a mode around 714 nm wavelength, the thickness of the waveguide needs to exceed 350 nm for all the cases studied in Fig. 3. Due to the relatively smaller ordinary index of 1.74 in the x-direction, only the fundamental TE1 mode can sustain in this waveguide design even with thickness as large as 1000 nm. For a homogeneous waveguide, mode hybridization and conversion can be observed when the thickness approaches 900 nm (Fig. 3a-3b). Such effects absent from the birefringence case within the studied thickness range.

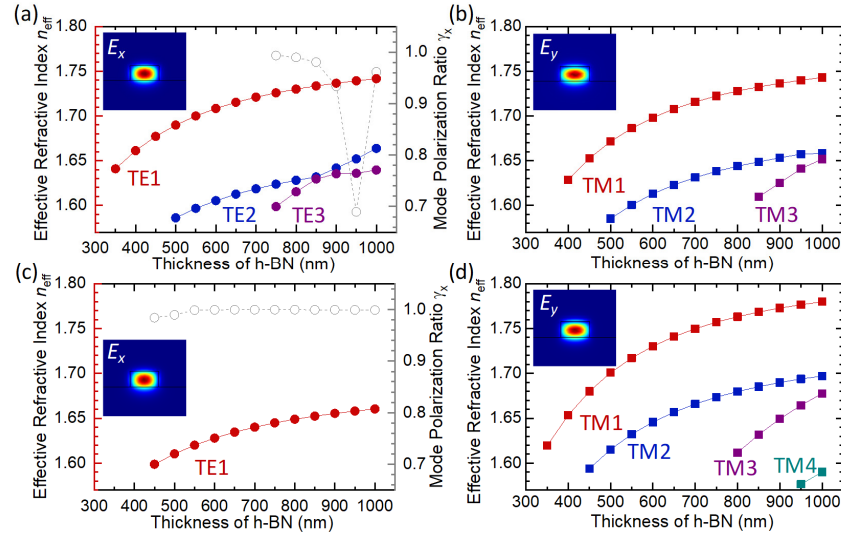


Fig. 3. Simulation of effective refractive index and representative mode shapes at a working wavelength of 714 nm for 1- μ m width h-BN ridge waveguide with varied thickness, by assuming (a-b) a normal refractive index of 1.8 or (c-d) birefringence indices of 1.72 and 1.84, respectively.

3. Conclusion

In this work, we have characterized the optical contrast and optical confinement of h-BN photonic devices at the wavelength corresponding to the quantum emission wavelength. The influence of the dielectric environment and the birefringence of h-BN have been investigated and will serve as a stepping stone toward the realization of integrated quantum photonic circuit based on 2D h-BN.

4. References

- [1] Y. Kubota, K. Watanabe, O. Tsuda, and T. Taniguchi, "Deep ultraviolet light-emitting hexagonal boron nitride synthesized at atmospheric pressure," *Science* **317**, 932–934 (2007).
- [2] L. Song, L. Ci, H. Lu, P. B. Sorokin, C. Jin, J. Ni, A. G. Kvashnin, D. G. Kvashnin, J. Lou, B. I. Yakobson, and P. M. Ajayan, "Large scale growth and characterization of atomic hexagonal boron nitride layers," *Nano Lett.* **10**, 3209–3215 (2010).
- [3] X.-Q. Zheng, J. Lee, and P. X.-L. Feng, "Hexagonal boron nitride nanomechanical resonators with spatially visualized motion," *Microsyst. Nanoeng.* **3**, 17038 (2017).
- [4] S. Dai, Z. Fei, Q. Ma, A. S. Rodin, M. Wagner, A. S. McLeod, M. K. Liu, W. Gannett, W. Regan, K. Watanabe, T. Taniguchi, M. Thiemens, G. Dominguez, A. H. Castro Neto, A. Zettl, F. Keilmann, P. Jarillo-Herrero, M. M. Fogler, and D. N. Basov, "Tunable phonon polaritons in atomically thin van der Waals crystals of boron nitride," *Science* **343**(6175), 1125–1129 (2014).
- [5] T. T. Tran, K. Bray, M. J. Ford, M. Toth, and I. Aharonovich, "Quantum emission from hexagonal boron nitride monolayers," *Nat. Nanotechnol.* **11**, 37 (2016).
- [6] S. Kim, J. E. Fröch, J. Christian, M. Straw, J. Bishop, D. Totonjian, K. Watanabe, T. Taniguchi, M. Toth, and I. Aharonovich, "Photonic crystal cavities from hexagonal boron nitride," *Nat. Commun.* **9**, 2623 (2019).
- [7] Y. Wang, V. Zhou, Y. Xie, X.-Q. Zheng, and P. X.-L. Feng, "Optical contrast signatures of hexagonal boron nitride on a device platform," *Opt. Mater. Express* **9**, 1223–1232 (2019).
- [8] I. Aharonovich, D. G. Englund, and M. Toth, "Solid-state single-photon emitters," *Nat. Photonics* **10**, 631 (2016).