Supporting Information for

Internal nanostructure diagnosis with hyperbolic phonon polaritons in hexagonal boron nitride

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1. Simulation of hyperbolic phonon polaritons in hexagonal boron nitride with/without the internal defect

Collective electromagnetic modes can be identified with the maxima of dissipation, that is the imaginary part of the complex reflectivity r_p (q, ω)[1]. Our system consists five layers: top hBN, air gap, bottom hBN, SiO_2 and Si for the defective hBN part, and three layers: hBN, SiO_2 and Si for the pristine hBN part. The complex r_p can be derived from Fresnel equations for these multilayer system[2]:

$$r_{p_{air\_hBN\_interface}} = \frac{\varepsilon_{hBN\_z} k^z_{air} - \varepsilon_{air} k^z_e}{\varepsilon_{hBN\_z} k^z_{air} + \varepsilon_{air} k^z_e} \quad \text{(S1)}$$

$$r_{p_{hBN\_SiO2\_interface}} = \frac{\varepsilon_{SiO2} q^z_e - \varepsilon_{hBN\_z} q^z_{SiO2}}{\varepsilon_{SiO2} q^z_e + \varepsilon_{hBN\_z} q^z_{SiO2}} \quad \text{(S2)}$$

$$r_{p_{SiO2\_Si\_interface}} = \frac{\varepsilon_{Si} q^z_{SiO2} - \varepsilon_{SiO2} q^z_{Si}}{\varepsilon_{Si} q^z_{SiO2} + \varepsilon_{SiO2} q^z_{Si}} \quad \text{(S3)}$$

$$r_{p_{SiO2}} = \frac{r_{p_{hBN\_SiO2\_interface}} + r_{p_{SiO2\_Si\_interface}} e^{i2q^z_{SiO2} d_{SiO2}}}{1 + r_{p_{hBN\_SiO2\_interface}} r_{p_{SiO2\_Si\_interface}} e^{i2q^z_{SiO2} d_{SiO2}}} \quad \text{(S4)}$$

where ε is the permittivity along the indicated axis in each layer and q represents the directional momentum of the photon in each layer. The subscript "*e*" stands for "extraordinary ray" of hBN which is optically uniaxial.

By tracking the maxima of complex reflectivity r_p (q, ω), we can simulate the hyperbolic phonon polaritons in Figures 2 and 3 of the main text.

2. Numerical modeling of polaritons and reflection, transmission and scattering

Numerical modelling of polaritons in hBN was performed using COMSOL Multiphysics. For this purpose, we designed a model of the cross-section of the hBN slab with a defect, as shown in Fig. 4C in the main text. The lowest-order hBN polaritons[2, 3] were excited from the left-side of hBN Region 1 using a numerical port (Port 1)[4]. Upon reaching the interior defect, the polariton energy get transmitted into hBN Region 2, reflected back to hBN Region 1 and scattered into higher-order polaritons. The output ports (Port 1 and Port 2 at the right-side of hBN Region 2) were configured to receive only the lowest-order mode: we performed the simulation on the hBN slab with a large lateral size such that only the lowest-order hBN polaritons can reach these ports while the higher-order polaritons get damped.

To obtain the Reflection R and Transmission T at the defect, we applied the same procedure as in Ref. [4]. Briefly, hBN Region 1 and 2 support polaritons with effective indexes $n_i = n_i' - jn_i''$

(n_i', $n_i'' > 0$ where i =1, 2 is the region/port number), the scattering parameters at the defect: $\tilde{S}_{ij}$, can be evaluated from the scattering parameters at the ports, S_{ij}, as[5]:

$$\tilde{S}_{ii} = S_{ii}e^{j2k_0 n_i L_i}$$

$$\tilde{S}_{ij} = S_{ij}e^{jk_0(n_i L_i + n_j L_j)},$$

where $k_0 = \omega / c$ is the free-space photon momentum and L_i is the distance between Port i and the defect. The reflection and transmission coefficients are:

$$R = |S_{11}|^2,$$

$$T = |S_{21}|^2.$$

The energy scattered into higher-order polaritons can be obtained with $S = 1 - R - T$.

References

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