Electronic Supplementary Material (ESI) for Nanoscale.

Supporting information for

Sandwiched graphene/hBN/graphene photonic crystal fiber with high electro-optical modulation depth and speed

Xu Cheng[#], Xu Zhou[#], Langyi Tao[#], Wentao Yu[#], Can Liu, Yi Cheng, Chaojie Ma, Nianze Shang, Jin Xie, Kaihui Liu[*], Zhongfan Liu[*]

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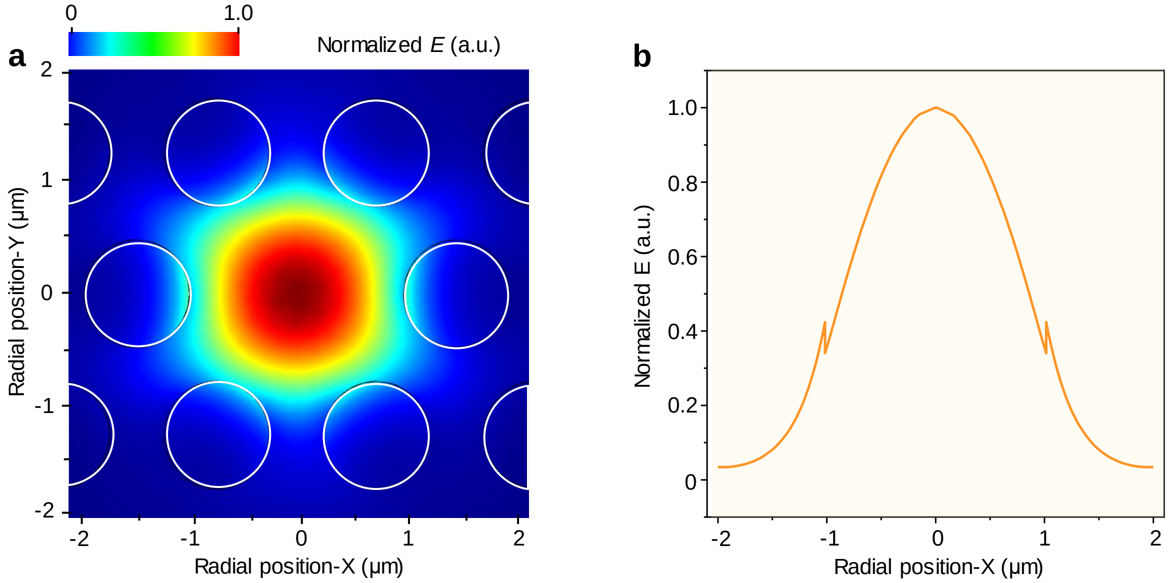

Fig. S1 | Electric field distribution in bare PCF. (a) The normalized calculated electric field distribution of the fundamental guided mode via finite element method. White circles highlight the air holes in the bare PCF with the same dimension as Fig. 1b in text. **(b)** The normalized electric field intensity of light in bare PCF along radial position-X at the radial position-Y equal to zero. It demonstrates that the transmitted light is confined in the solid fiber core.

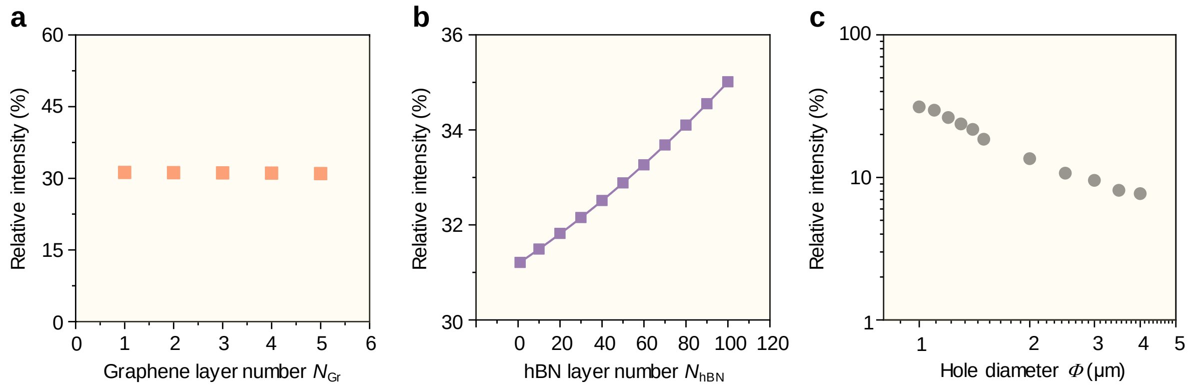

Fig. S2 | Electric field relative intensity in different Gr/hBN/Gr PCF structures. If not specifically mentioned, the layer number of graphene and hBN are both one, and the hole diameter and pitch are 1 μm and 1.516 μm, respectively. **(a)** Relative intensity (ratio of light intensity at innermost graphene position to that at core center) approximately remains unchanged as the graphene layer number increases, indicating a stable light-graphene interaction and linear dependence of light absorption on layer number. **(b)** Relative intensity increases nonlinearly with the hBN layer number to prove a nonlinear dependence of light-graphene interaction on layer number. The simulated data is fitted well with a parabolic function. **(c)** Relative intensity decreases exponentially with the hole diameter Φ (keeping single mode transmission > 1260 nm) to imply an exponential dependence of light-graphene interaction on Φ.

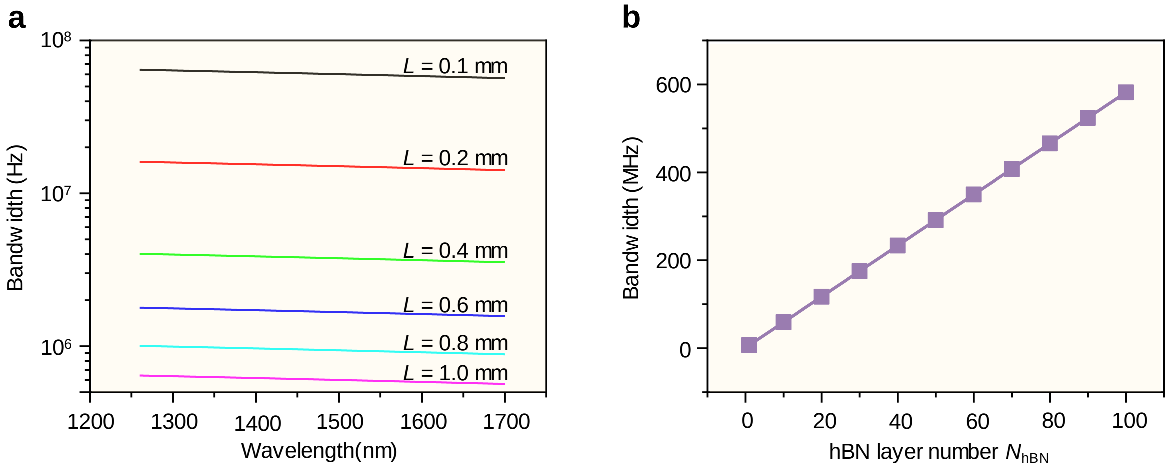

Fig. S3 | Bandwidth dependence on wavelength and hBN layer number. (a) Bandwidth dependence on wavelength of incident light transmitting in Gr/hBN/Gr PCF modulator. It shows that bandwidth slightly decreases with the wavelength (in one-to-one correspondence with carrier concentration) on condition of the fiber length changing from 0.1mm to 1.0 mm, indicating a nearly uniform operation bandwidth in large wavelength range. Layer number of graphene and hBN are set as 1 and 100 respectively, under the same conditions as Fig. 4b. **(b)** Bandwidth dependence on hBN layer number. Bandwidth increases nearly linearly with the hBN layer number from 6 MHz to 600 MHz, due to the smaller capacitance of Gr/hBN/Gr with thicker hBN film. Here the fiber length is set as 0.1 mm, the carrier concentration n ~9.7×10^{12} cm^{-2}, and the working wavelength at 1550 nm.

Note S1. The drive voltage related with Fermi Level

The Fermi level of graphene is expressed as

$$E_{\mathrm{F}} = \hbar|v_{\mathrm{F}}|\sqrt{\pi n}, \tag{1}$$

where the Fermi velocity of graphene $|v_{\mathrm{F}}| = 1.1\times10^{6}$ m/s, $\hbar$ is the reduced Planck constant, π is the circular constant and n is the carrier concentration[1].

While in our equivalent circuit, the drive voltage V_{dr} is the sum of the voltage drops caused by the quantum capacitance of graphene and the hBN film in the Gr/hBN/Gr capacitor, that is

$$V_{\mathrm{dr}} = 2\cdot\frac{\hbar|v_{\mathrm{F}}|\sqrt{\pi n}}{e} + \frac{ne}{C_{\mathrm{E}}}, \tag{2}$$

where $C_{\mathrm{E}} = \varepsilon/d$, e, d and ε are the capacitance of the capacitor, electron charge, the thickness and permittivity of the hBN layers, respectively. Therefore, the V_{dr} related with E_{F} can be deduced from the two formulas above as

$$V_{\mathrm{dr}} = \frac{2E_{\mathrm{F}}}{e} + \frac{ed}{\pi\varepsilon\hbar^{2}v_{\mathrm{F}}^{2}}\cdot E_{\mathrm{F}}^{2}. \tag{3}$$

When E_{F} is located at the energy level of 0.49 to 0.36 eV (corresponding 1260 to 1700 nm of incident photon) with hBN thickness d = 34 nm, the drive voltage just needs ~28.3 to ~15.6 V which is a relatively low intrinsic operating voltage compared to the conventional lithium niobate crystal modulator.

Note S2. The bandwidth of Gr/hBN/Gr PCF modulator

The bandwidth of Gr/hBN/Gr PCF modulator is given by $f = 1/(2\pi RC)$, where R is the effective total resistance and C is the capacitance corresponding to the equivalent circuit (Fig. 4a in text). Obviously, the R and C is related with carried concentration (n) of graphene. Considering the scattering effects[2-4], the sheet resistance R_s and total resistance R can be written as

$$R_s = R_{s\infty} + \frac{1}{ne\mu_C + 1/R_{s0}}, \tag{4}$$

$$R = 2R_s \cdot \frac{L}{W}, \tag{5}$$

where $R_{s\infty}$, μ_C, and R_{s0} are respectively the resistance induced by the short-range scattering when carried concentration approaches infinity ($n \rightarrow \infty$), the carrier concentration-independent carrier mobility and the residual resistance at Dirac point of graphene. The influence of the hBN substrate on graphene plates is reflected on the sheet resistance of graphene[3]. L is the fiber length and W is the perimeter of the holes of PCF.

The total effective capacitance per unit area is the capacitance of the Gr/hBN/Gr structure C_E and the quantum capacitance $C_Q \approx \frac{2e^2}{\hbar v_F \sqrt{\pi}} \sqrt{n}$ of graphene in series[5], the total capacitance can be written as

$$C = \frac{1}{\frac{2}{C_Q} + \frac{1}{C_E}} \cdot S = \frac{LW}{\frac{\hbar v_F \sqrt{\pi}}{e^2 \sqrt{n}} + \frac{d}{\varepsilon}}. \tag{6}$$

From the expression of R and C, we can then obtain the bandwidth as following

$$f = \frac{d + \frac{\varepsilon \hbar v_F \sqrt{\pi}}{e^2} \cdot \frac{1}{\sqrt{n}}}{4\pi\varepsilon L^2 \left(R_{s\infty} + \frac{1}{ne\mu_C + \sigma_0}\right)} = \frac{d + 0.23 \cdot \frac{1}{\sqrt{n}}}{L^2 \left(4.4 + \frac{1.4\times10^{17}}{n + 3.3\times10^{15}}\right)} \times 10^8. \tag{7}$$

Using the experimental data ($R_{s\infty} \approx 120\ \Omega$, $\mu_C \approx 16000\ \mathrm{cm^2/(V{\cdot}s)}$ and $\sigma_0 \approx 3.25\times10^{-4}\ \Omega^{-1}$) from Ref. 3, we can map the 3-dimensinal relationship between carrier concentration, fiber length and bandwidth (as shown Fig. 4b in text) as the hole diameter is 1 μm, hole pitch is 1.516 μm, hBN layer number is 100 (thickness d = 34 nm) and graphene layer number is 1.

Table. Material parameters used in calculation

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Material Parameters	Value
Graphene refractive index (1550 nm)[6]	2.934
hBN refractive index (1550 nm)[7]	1.8
$R_{s\infty}$[3]	120 Ω
μ_C[3]	16000 $cm^2/(V \cdot s)$
R_{s0}[3]	3077 Ω

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