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Supplementary Materials for

Intrinsically core-shell plasmonic dielectric nanostructures with ultrahigh refractive index

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The PDF file includes:

B-spline model

The refractive index and dielectric constants of flat BSTS crystals were measured using spectroscopic ellipsometry. The spectroscopic data of metallic surface was fitted using the B- splines, which is a basic model for the parameterization in spectroscopic ellipsometry. The B-spline was initially developed by Johs and Hale from J.A. Woollam Co. Inc. It is a fast and simple-to-apply method to accurately determine thickness and dielectric constants of thin films. It does not require prior knowledge about the thin films and demonstrates high flexibility for metallic materials.

B-splines (Basis-splines) are a recursive set of polynomial splines. Their basis function $\mathrm{B}_i^k(x)$ is defined by:

$$\mathrm{B}_i^0(x) = \begin{cases} 1, & t_i \le x \le t_{i+1} \\ 0, & \text{otherwise} \end{cases} \quad (1)$$

$$\mathrm{B}_i^k(x) = \left(\frac{x-t_i}{t_{i+k}-t_i}\right)\mathrm{B}_i^{k-1}(x) + \left(\frac{t_{i+k+1}-x}{t_{i+k+1}-t_{i+1}}\right)\mathrm{B}_{i+1}^{k-1}(x) \quad (2)$$

where k is the degree of the B-spline and i the index for the knots t_i. Equation (1) defines the degree 0 B-spline basis function. Higher degree B-spline basis functions are constructed using the recursion relation (2).

A spline curve $S(x)$ is then constructed as a linear sum of n basis functions (3). Then, the total spline curve $S(x)$, representing the dielectric function of the material, is given by:

$$S(x) = \sum_{i=1}^{n} C_i B_i^k(x) \quad (3)$$

where C_i is the B-spline coefficient. Then, the dielectric function of the surface layer can be expressed as,

$$\varepsilon_2(\omega) = \sum_{i=1}^{n} C_i \, B_i^k(\omega) \quad (4)$$

$$\varepsilon_1(\omega) = \varepsilon_1(\infty) + \sum_{i=1}^{n} C_i \, \emptyset_i^k(\omega) \quad (5)$$

where $\emptyset_i^k(\omega) = \frac{2}{\pi} P \int_0^\infty \frac{\omega' B_i^k(\omega')}{\omega'^2 - \omega^2} d\omega'$

Tauc-Lorentz model

The Tauc-Lorentz model was used to fit the ellipsometry data of the insulating bulk of BSTS crystals. The model is a powerful tool to parameterize the optical absorption of dielectric bulk materials, which was proposed by Jellison and Modine. The dielectric function of Tauc-Lorenz dispersion formula can be expressed as,

$$\varepsilon_2(E) = \frac{AE_0C(E-E_g)^2}{(E^2-E_0^2)^2+C^2E^2}\frac{\Theta(E-E_g)}{E} \quad (6)$$

$$\varepsilon_1(E) = \varepsilon_\infty + \frac{2}{\pi}P\int_{E_g}^{\infty}\frac{\xi\varepsilon_2(\xi)}{\xi^2-E^2}d\xi \quad 7)$$

where $\Theta(x) = 0$ for $x < 0$ and 1 for $x > 0$. E_g = 0.25 eV, E_0 = 1.94 eV, $\varepsilon_\infty = 0$, A = 65.9, and C = 1.94 are the fitting parameters, which correspond to the BSTS band gap, peak in joint density of states, high frequency dielectric constant, amplitude of absorption peak, and broadening factor, , respectively.

Crystal structures of BSTS

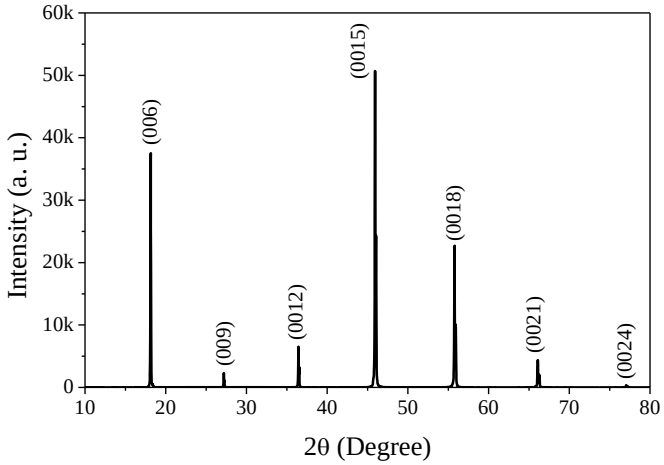

fig. S1. XRD of BSTS bulk crystals with growing orientation along (001). The diffraction peaks in the XRD indicate the high quality of our bulk BSTS crystal samples.

Morphology of BSTS nanocone arrays

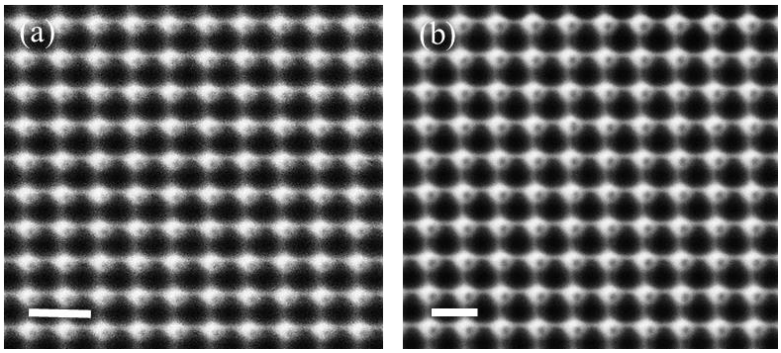

fig. S2. SEM images of topological insulator BSTS nanocone arrays. (a) BSTS nanocone arrays with d = 300 nm and p = 600 nm, (b) BSTS nanocone arrays with d = 400 nm and p = 800 nm. The scale bar in both (a) and (b) is 1000 nm.

FDTD simulation of plasmonic absorption

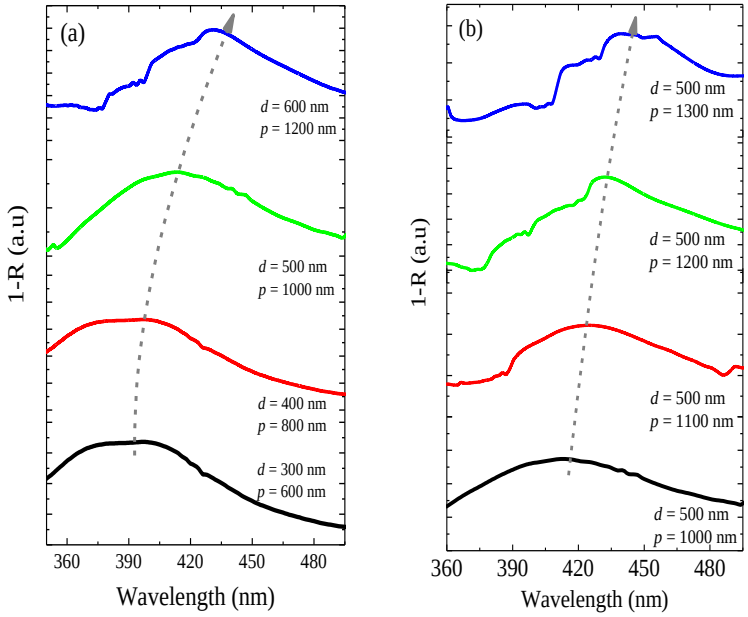

fig. S3. FDTD simulation of plasmonic absorption spectra in BSTS nanocone arrays. (a) Simulated absorption spectra of BSTS nanocone arrays with different base diameters of *d* and periods of *p*. *d* changes from 300 nm to 600 nm. *p* changes from 600 nm to 1200 nm. (b) FDTD simulation of absorption spectra of BSTS nanocone arrays with *d* = 500 nm and different values of *p* ranging from 1000 nm to 1300 nm.

FDTD simulation of field distribution

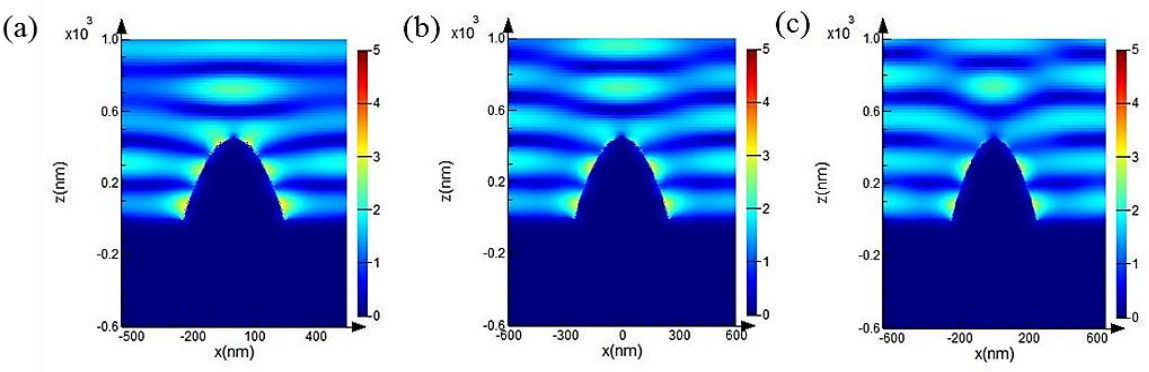

fig. S4. FDTD simulation of the electromagnetic field distribution in BSTS nanocone arrays. *d* = 500 nm and *p* changes from 1100 nm to 1300 nm. (a) The nanocone arrays with *p* = 1100 nm at a wavelength of 440 nm, (b) The nanocone arrays with *p* = 1200 nm at a wavelength of 450 nm, and (c) The nanocone arrays with *p* = 1300 nm at a wavelength of 460 nm.

Comparison of plasmonic absorption

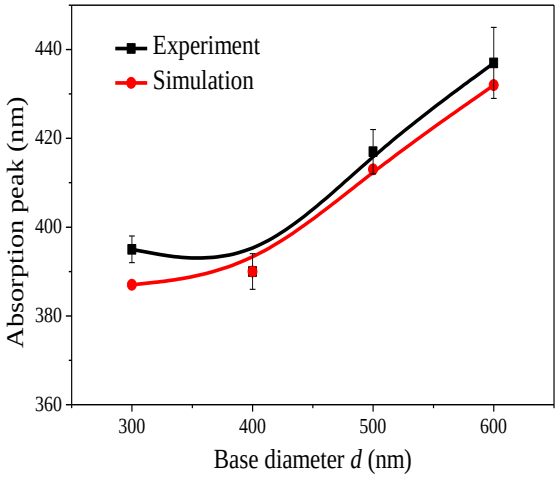

fig. S5. Wavelengths of the absorption resonance peaks as a function of base diameter *d* of BSTS nanocones. The period *p* of nanocone arrays ranges from 600 nm to 1200 nm. The black curve represents the experimental data and the red curve represents the FDTD simulation data. The distinction between experimental data and simulated data may result from the roughness of nanocones and BSTS basements.