Improved piezoelectricity and elasticity of Ce-doped $BaTiO_3$ nanofibers—towards energy harvesting application

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Contents:

Calculation of the Theoretical of elastic modulus

The elastic modulus can be calculated from the F-D curves obtained from AFM. The distances shown in the F-D curves are the sum of the indenter (the combination of the cantilever, probe and substrate) displacement (x) and sample indentation (δ). The total effective stiffness, k_{eff}, of the whole AFM contact is composed of two contributions in series: the indenter stiffness, k_i, and the tip-sample contact stiffness, k_s. k_i is obtained via the slope of the F-d data of the silicon substrate, where $k_s = dF/d\delta$. The slope of the F-d data after the AFM tip contacting the sample surface is employed to calculate the k_{eff}. The fiber stiffness can be calculated using the following relation: [1]

$$k_s = \frac{k_{eff} k_i}{k_i - k_{eff}} \tag{1}$$

From which we can calculate the δ value. The obtained k_i is 0.089 N/m, k_{eff} are 0.088 N/m and 0.087 N/m with Ce/Ba atomic ratio of 0.0% and 0.6%, respectively, as the slopes can be obtained from the F-d curves. The calculated k_s from Equation (1) are 7.832 N/m (the Ce/Ba atomic ratio is 0.0) and 3.8715 N/m (the Ce/Ba atomic ratio is 0.6%), respectively. The δ values can be estimated from k_s to be 1.28 nm (0.0) and 2.58 nm (0.6%) when the applied force is 10 nN.

The elastic modulus of the fibers can be estimated using the following expression for an elastic sphere plane contact described by a Hertz model: [2, 3]

$$F = \frac{4ER^{1/2}\delta^{3/2}}{3(1-\nu^2)} \tag{2}$$

$$\frac{1}{R} = \frac{1}{R_{tip}} + \frac{1}{R_s} \tag{3}$$

where F is the loading force, E is the Young's modulus of the fiber, δ is the indentation, ν is the Poisson ratio of the fiber (0.3), [4] R is the effective radius of tip-sample system, and R_{tip} is the tip radius (R_{tip}=2 nm), R_s is the fiber radius. The estimated elastic modulus of the fibers with Ce/Ba atomic ratios of 0.0% and 0.6% are 3.37 GPa and 1.18 GPa, respectively, when the applied load is 10 nN.

Supplementary Figures

Figure S1 Raman spectra of Ce-doped BTO nanofibers with different cerium concentration.

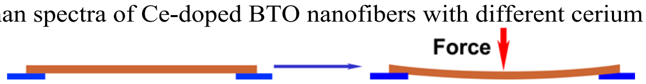

Figure S2 Schematic diagram of the testing procedure.

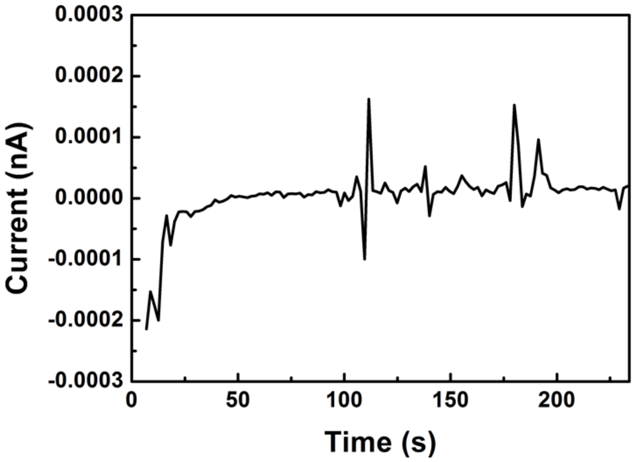

Figure S3 Output current of the energy harverster which contain no BTO nanofibers

Figure S4 Output signals of the energy harvesters fabricated by Ce-doped BTO nanofibers: output voltage signals with Ce/Ba atomic ratios of (a) 0.2%, (c) 0.4%, and (e) 0.8%; output current signals with Ce/Ba atomic ratios of (b) 0.2%, (d) 0.4%, and (f) 0.8%

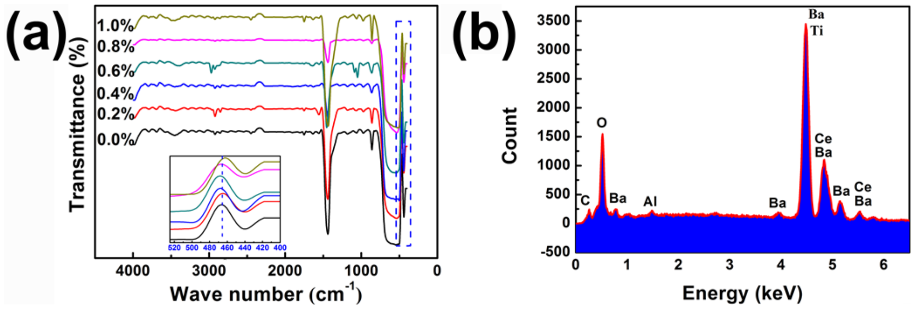

Figure S5 (a) FTIR spectra of Ce-doped BTO nanofibers with different cerium concentration. The broad band at 3400 cm^{-1} is assigned to the asymmetric vibration of O-H stretching of water molecules adsorbed. [5] The peaks at 2350 cm^{-1}, 1750 cm^{-1}, 1430 cm^{-1} and 860 cm^{-1} are assigned to the contaminants of the CO_3^{2-} group in $BaCO_3$. [6] The absorbance bands at wavenumbers 2920 cm^{-1} and 2845 cm^{-1} correspond to CH_2 and CH_3 stretching, respectively. (b) EDAX analysis of Ce-doped BTO nanofibers. The molar ratio of Ce to Ba is 0.006.

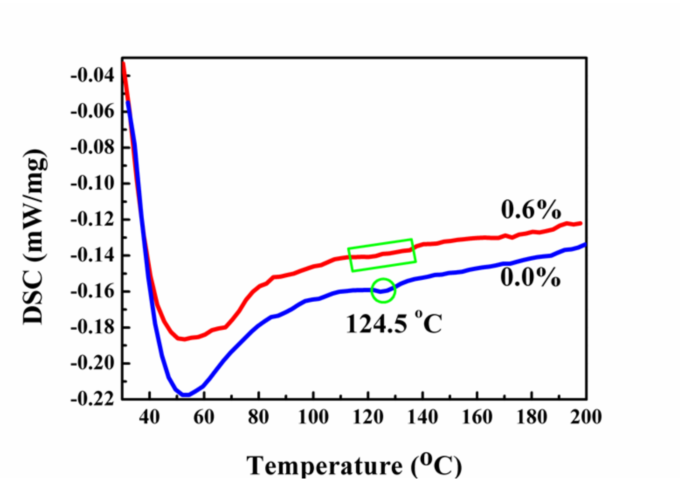

Figure S6 Differential scanning calorimetry (DSC) curves of the BTO nanofibers with Ce/Ba atomic ratios of 0.0% and 0.6%, respectively.

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