Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary materials

The Raman spectroscopy was used to analyze the relationship between dielectric properties and crystal structure of BNT-AGx ceramics in this work. As shown in Table S1, for all 8d and 4c wyckoff positions with one 4a position, BNT-AGx structure belonged to the space group Pbnm and had 8 types vibration modes in lattice: A_g, A_u, B_{1g}, B_{1u}, B_{2g}, B_{2u}. B_{3g} and B_{3u} based on the group theory and D_{2h} point group. The irreducible representations for the structure were obtained by the following equation[1]:

$$n_m = \frac{1}{h}\sum_R \chi(R)U(R)(\pm 1 + 2\cos\theta_R)$$

Here, n_m was the number of vibrational modes with a symmetry presented by the mth irreducible representation, the h=8 was derived from the order of vector group that made up of all symmetry elements R, $\chi(R)$ was the reducible representation of R, U(R) was the number of atoms under the symmetry operations of space group, and $(\pm 1+2\cos\theta_R)$ was the trace of the matrix R.

Table 1 Date used for irreducible representation analysis

D_{2h}	R								Functions	Number of vibration modes
	E	C_2^z	C_2^z	C_2^z	I	σ_{xy}	σ_{xz}	σ_{yz}		
A_g	1	1	1	1	1	1	1	1	x^2, y^2, z^2	71
B_{1g}	1	1	-1	-1	1	1	-1	-1	xy, J_z	55
B_{2g}	1	-1	1	-1	1	-1	1	-1	xz, J_y	71
B_{3g}	1	-1	-1	1	1	-1	-1	1	yz, J_x	55
A_u	1	1	1	1	-1	-1	-1	-1	-	58
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	74
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	58
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	74
U(R)	172	0	0	0	4	64	0	0		
$\pm 1+2\cos\theta_R$	3	-1	-1	-1	-3	1	1	1		

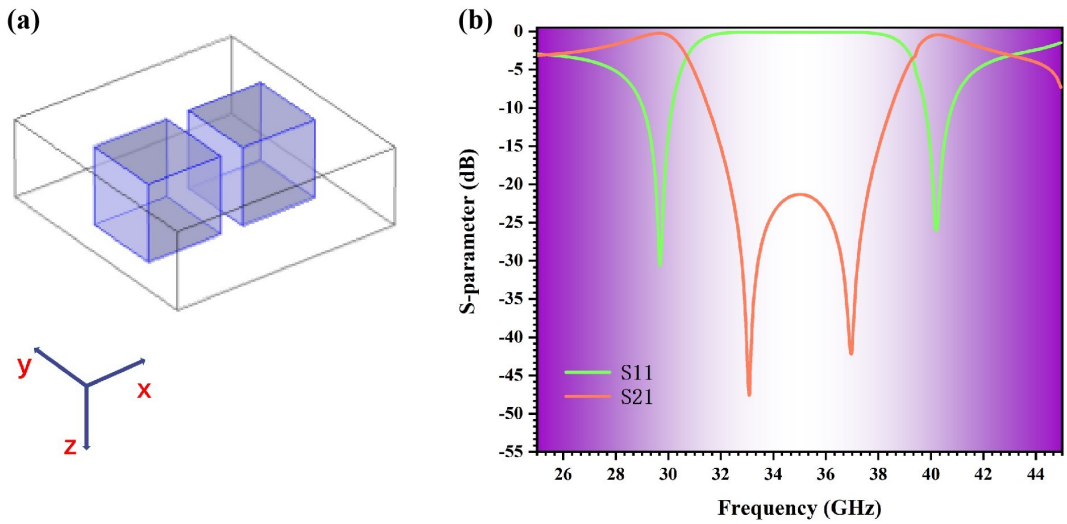

Fig. S1 Simulated results of (a) the BNT-AGx reflective filter unit cell structure and (b) the S-parameter.

Here, we utilized a dimer structure (1×1×1 mm^3, in Fig. S1(a)) embedded in FR4 (p=3 mm, the distance between two blocks was 1 mm) to achieve the mode coupling between BNT-AGx blocks, forming a broadband reflective filter. The transmission stop-band was about 7 GHz (@ 10 dB) with low insertion loss about 0.5 dB, as shown in Fig. S1(b).

Reference

[1] S. R. Zhang, Z. X. Fang, Z. Xiong, B. Tang, C. T. Yang, J. Alloys Compd. **2017**, 723, 580.