Supplementary Material

A comprehensive study on low temperature sintering and microwave/terahertz dielectric properties of BaO-P_2O_5 binary ceramics

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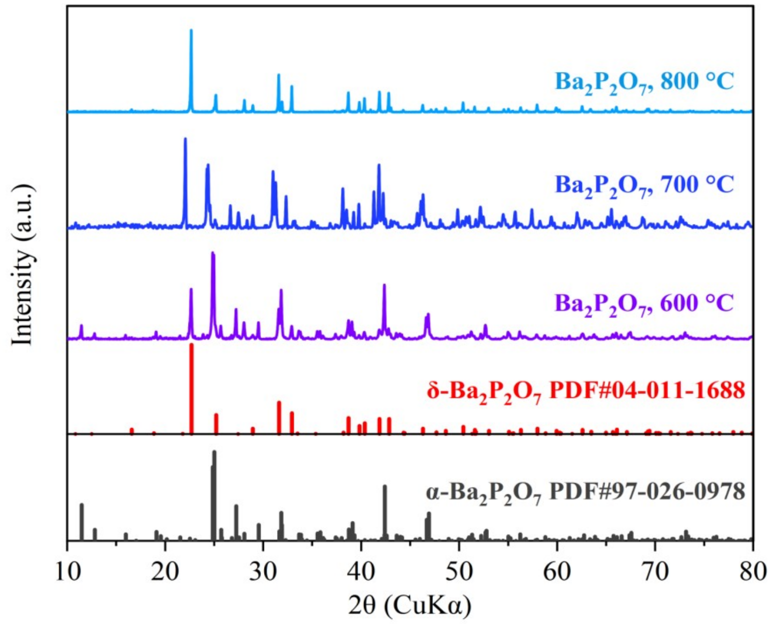

Fig. S1 XRD patterns of $Ba_2P_2O_7$ calcined at 600 ℃, 700 ℃, 800 ℃ for 4 h, respectively.

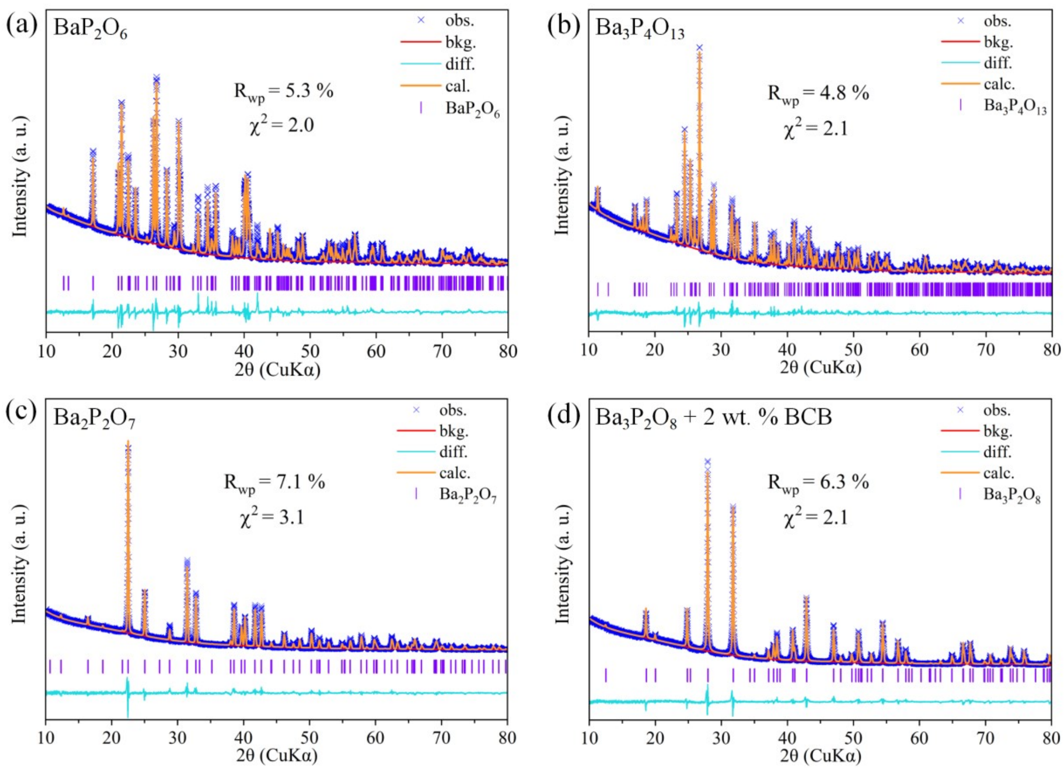

Fig. S2 Rietveld refinement pattern of (a) BaP_2O_6, (b) $Ba_3P_4O_{13}$, (c) $Ba_2P_2O_7$ and (d) $Ba_3P_2O_8$ + 2 wt. % BCB sintered at their respective optimal sintering temperatures.

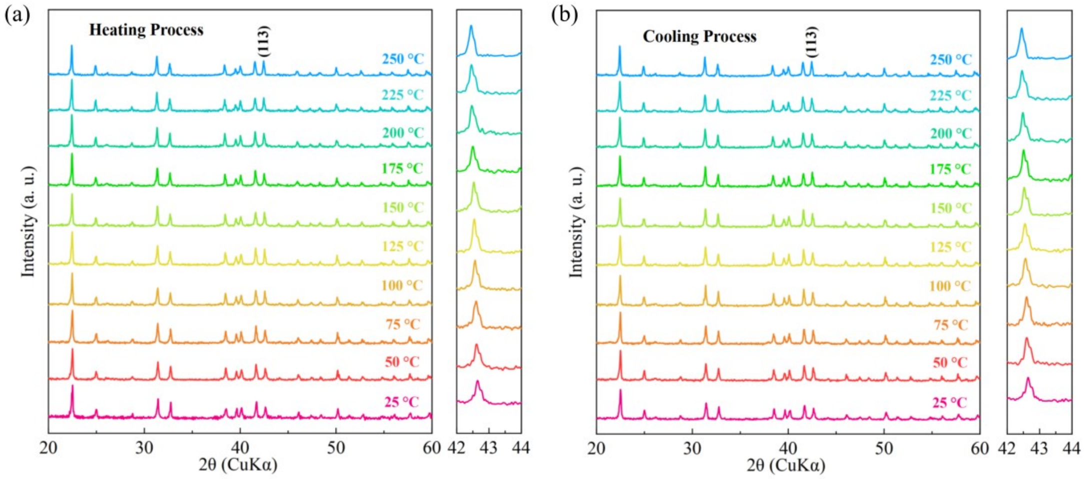

Fig. S3 Insitu high-temperature XRD patterns and disparity in (113) X-ray diffraction peaks for $Ba_2P_2O_7$ sintered at 1100 °C: (a) heating process, (b) cooling process.

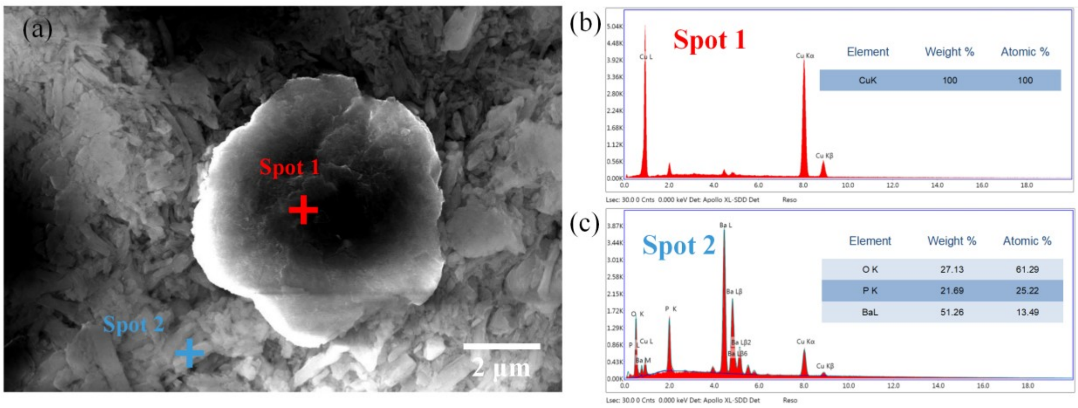

Fig. S4. The BSE and EDS results for BaP_2O_6 ceramics co-fired with Cu powders

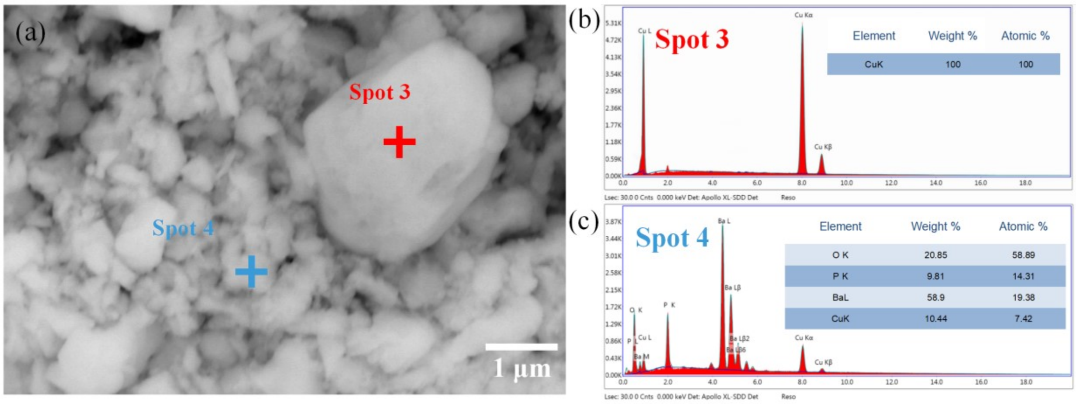

Fig. S5 The BSE and EDS results for $Ba_3P_2O_8$ + 2 wt. % BCB ceramics co-fired with Cu powders.

Table S1 Lattice parameters and refinement result of BaP_2O_6 ceramic sintered at 800 °C.

Atom	*x*	*y*	*z*
Ba1	0.2635(1)	0.1252(6)	0.1982(3)
P1	0.7176(1)	0.3534(8)	0.2225(4)
P2	0.2234(1)	0.4037(7)	0.4272(1)
O1	0.3933(5)	0.3467(2)	0.2674(1)
O2	0.9038(8)	0.3667(2)	0.3953(2)
O3	0.6910(4)	0.4383(1)	0.1392(4)
O4	0.8194(4)	0.2405(3)	0.1290(4)
O5	0.7385(3)	0.0124(2)	0.1213(2)
O6	0.8118(6)	0.1244(1)	0.3860(4)

a = 4.5001(2) Å, b = 13.3981(9) Å, c = 8.3419(5) Å, V = 502.95(4) $Å^3$, R_{wp} = 5.3 %, χ^2 = 2.0

Table S2 Lattice parameters and refinement result of $Ba_3P_4O_{13}$ ceramic sintered at 840 °C.

Atom	*x*	*y*	*z*
Ba1	0	0	0
Ba2	0.6475(4)	−0.4135(8)	0.2275(4)
P1	−0.0005(7)	0.2050(2)	−0.4610(8)
P2	0.3427(7)	0.1902(6)	0.1939(4)
O1	0.0847(2)	0.3063(1)	0.1161(1)
O2	0.5292(2)	0.2939(2)	0.1395(1)
O3	0.2469(1)	0.2337(1)	0.4015(1)
O4	0.4143(1)	−0.0319(1)	0.1835(1)
O5	−0.0241(5)	0.2501(4)	−0.3112(3)
O6	0.0937(5)	0.1805(4)	−0.3001(3)
O7	−0.2677(5)	0.2893(4)	0.4585(3)
O8	−0.2313(5)	0.3628(4)	−0.5113(3)
O9	−0.0901(4)	0.0536(4)	0.4597(28)
a = 5.6909(1) Å, b = 7.2411(7) Å, c = 8.0137(5) Å, α = 83.6186(3) °, β = 75.9522(5) °, γ = 70.4811(7) °, V=301.78(2) $Å^3$, R_{wp} = 4.8 %, χ^2 = 2.1			

Table S3 Lattice parameters and refinement result of $Ba_2P_2O_7$ ceramic sintered at 1100 °C.

Atom	*x*	*y*	*z*
Ba1	0.3819(2)	0.3819(2)	1/2
Ba2	0.2896(2)	0	0
P1	0	0	0.3005(8)
P2	2/3	1/3	0.2242(1)
O1	0.8520(5)	0	0.2618(1)
O2	0.5123(8)	0.1849(2)	0.3103(5)
O3	−0.0465(5)	0	1/2
O4	0.3117(1)	0.5628(2)	0
a = 9.4065(3) Å, c = 7.0728(2) Å, V = 541.97(5) Å^3, R_{wp} = 7.1 %, χ^2 = 3.1			

Table S4 Lattice parameters and refinement result of $Ba_3P_2O_8$ + 2 wt. % BCB ceramic sintered at 800 °C.

Atom	*x*	*y*	*z*
Ba1	0	0	0.4052(9)
Ba2	0	0	0
P1	0	0	0.2094(6)
O1	0	0	0.3359(1)
O2	0.8460(5)	0.1539(5)	0.4331(2)
a = 5.5968(5) Å, c = 20.9700(2) Å, V = 568.87(5) Å^3, R_{wp} = 6.3 %, χ^2 = 2.1			

Table S5 Phonon parameters determined from FTIR for $Ba_3P_2O_8$ ceramic. ($\Delta\varepsilon_j$ is the contribution of the *j*-th oscillator to the static permittivity)

Modes	$Ba_3P_2O_8$				
	ω_{oj}	ω_{pj}	γ_j	S_j	$\Delta\varepsilon_j$
1	77.468	80.843	6.5941	1.09	0.0851
2	136.93	223.48	12.505	2.66	0.0913
3	155.48	59.64	8.5312	0.147	0.0549
4	199.79	245.75	14.262	1.51	0.0714
5	227.75	88.196	57.809	0.15	0.254
6	554.34	267.51	6.8391	0.233	0.0123
7	927.3	64.479	4.8753	0.00484	0.00526
8	996.64	439.19	16.364	0.194	0.0164
9	1008.9	355.71	27.387	0.124	0.0271
10	1014	285.79	40.6	0.0794	0.04
11	1089	131.04	32.33	0.0145	0.0297
12	1100.8	101.76	222.82	0.00855	0.202
	$\varepsilon_\infty = 2.78$			$\varepsilon_0 = 9.00$	

Table S6. Phonon parameters determined from FTIR for $Ba_3P_2O_8$ + 2 wt. % BCB ceramic.

Modes	$Ba_3P_2O_8$ + 2 wt. % BCB				
	ω_{oj}	ω_{pj}	γ_j	S_j	$\Delta\varepsilon_j$
1	77.458	62.63	6.5485	0.654	0.0845
2	132.17	69.019	4.5943	0.273	0.0348
3	140.85	177.24	15.829	1.58	0.112
4	180.29	35.22	7.0113	0.0382	0.0389
5	204.82	189.89	11.43	0.859	0.0558
6	217.53	164.81	45.046	0.574	0.207
7	555.38	247.09	7.2396	0.198	0.013
8	927.51	48.985	3.9837	0.00279	0.0043
9	991.33	350.09	13.662	0.125	0.0138
10	1003.8	373.4	19.418	0.138	0.0193
11	1021.4	279.82	26.041	0.0751	0.0255
12	1059.7	95.182	34.019	0.00807	0.0321
13	1086.4	99.609	24.757	0.00841	0.0228
	$\varepsilon_\infty = 2.65$			$\varepsilon_0 = 7.18$	

Table S7 Comparisons of dielectric properties determined by THz-TDS and AVNA for BaP_2O_6 ceramic.

Methods	BaP_2O_6			
	ε'	ε''	tanδ	$Q\times f$ (GHz)
THz-TDS (@ 1 THz)	5.88	1.89×10^{-1}	3.21×10^{-2}	3.12×10^{4}
AVNA (@ 12.72 GHz)	6.23	4.63×10^{-3}	7.44×10^{-4}	1.71×10^{4}

Table S8 Comparisons of dielectric properties determined by THz-TDS and AVNA for $Ba_3P_4O_{13}$ ceramic.

Methods	$Ba_3P_4O_{13}$			
	ε'	ε''	tanδ	$Q\times f$ (GHz)
THz-TDS (@ 1 THz)	7.69	9.89×10^{-1}	1.29×10^{-1}	7.75×10^{3}
AVNA (@ 11.18 GHz)	7.70	6.06×10^{-3}	7.87×10^{-4}	1.42×10^{4}

Table S9 Comparisons of dielectric properties determined by THz-TDS and AVNA for $Ba_2P_2O_7$ ceramic.

Methods	$Ba_2P_2O_7$			
	ε'	ε''	tanδ	$Q\times f$ (GHz)
THz-TDS (@ 1 THz)	7.65	8.82×10^{-1}	1.15×10^{-1}	8.70×10^{3}
AVNA (@ 11.76 GHz)	7.90	2.57×10^{-2}	3.26×10^{-3}	3.64×10^{3}

Table S10 Design parameters of the proposed antennas.

Symbol	Value (mm)	Symbol	Value (mm)
L_1	50.00	h	3.71
D	9.08	t	0.035
w	2.00	sub_h	1.575
l	8.70	L_2	76.00
$l_{part\text{-}1}$	11.20	L_3	19.00
$l_{part\text{-}2}$	9.50	W	54.00
$l_{part\text{-}3}$	5.50	$l_{part\text{-}4}$	6.20
w_100	1.38	$l_{part\text{-}5}$	7.50
w_71	2.67	$l_{part\text{-}6}$	42.76
w_50	4.76	$l_{part\text{-}7}$	12.00
w_35	7.80	$l_{part\text{-}8}$	2.50