

Electronic Supplementary Material

Table S1 The structural parameters and reliability factors of the BNT–A ceramics ($0 \leq z \leq 2$) obtained by

Rietveld refinement

z	$z = 0$	$z = 0.25$	$z = 0.5$	$z = 0.75$	$z = 1$
T_{sinter} (°C)	1400	1350	1350	1350	1350
R_p (%)	4.02	3.98	4.01	4.18	4.29
R_{wp} (%)	5.25	5.17	5.23	5.49	5.68
χ^2	2.66	2.45	2.63	2.93	3.03
a (Å)	12.19124(16)	12.18444(16)	12.17973(16)	12.17451(17)	12.16943(17)
b (Å)	22.3083(3)	22.3007(3)	22.3006(3)	22.2973(3)	22.2973(3)
c (Å)	7.68919(9)	7.68810(9)	7.68559(9)	7.68375(10)	7.68093(10)
V (Å ³)	2091.19(5)	2089.03(5)	2087.52(5)	2085.82(5)	2084.19(5)
ρ_{calc} (g/cm ³)	5.751	5.752	5.752	5.752	5.751
ρ_{meas} (g/cm ³)	5.66	5.676	5.676	5.685	5.686
ρ_{rela} (%)	98.42	98.68	98.68	98.84	98.87
B(1)–O (Å)	1.9420(52)	1.9313(55)	1.9389(54)	1.9449(57)	1.9475(56)
B(2)–O (Å)	1.9605(62)	1.9577(63)	1.9529(60)	1.9542(65)	1.9481(65)
B(3)–O (Å)	1.9539(62)	1.9502(63)	1.9569(64)	1.9591(68)	1.9756(67)
B(4)–O (Å)	2.0020(59)	1.9978(61)	1.9912(62)	1.9923(65)	1.9865(62)
B(5)–O (Å)	1.9869(61)	1.9904(63)	1.9884(60)	1.9821(64)	1.9805(64)
A1(1)–O (Å)	2.6899(63)	2.6679(68)	2.6855(64)	2.6624(72)	2.6623(66)

A1(2)–O (Å)	2.7172(65)	2.7241(68)	2.7114(65)	2.7187(75)	2.7258(69)
A1(3)–O (Å)	2.6954(67)	2.7037(69)	2.7070(67)	2.6978(73)	2.7001(73)
A1(4)–O (Å)	2.7235(68)	2.7069(68)	2.7198(67)	2.7351(73)	2.7349(71)
A1(5)–O (Å)	2.6684(73)	2.6827(73)	2.6733(71)	2.6454(76)	2.6558(76)
A2(1)–O (Å)	3.1568(62)	3.1542(62)	3.1570(64)	3.1902(71)	3.2007(66)
A2(2)–O (Å)	3.1433(63)	3.1499(62)	3.1382(64)	3.1263(72)	3.0940(68)
avg(B–O) (Å)	1.9721(60)	1.9693(62)	1.9686(61)	1.9689(65)	1.9699(64)
avg(A1–O) (Å)	2.6989(67)	2.6971(69)	2.6994(67)	2.6919(74)	2.6958(71)
avg(A2–O) (Å)	3.1501(63)	3.1521(62)	3.1476(64)	3.1583(72)	3.1474(67)

<i>z</i>	<i>z</i> = 1.25	<i>z</i> = 1.5	<i>z</i> = 1.75	<i>z</i> = 2
<i>T</i> _{sinter} (°C)	1400	1350	1350	1400
<i>R</i> _p (%)	4.47	4.30	4.26	4.30
<i>R</i> _{wp} (%)	6.24	5.81	5.72	5.74
χ^2	3.44	3.05	3.37	3.26
<i>a</i> (Å)	12.16431(19)	12.16168(18)	12.16032(18)	12.15894(19)
<i>b</i> (Å)	22.2957(4)	22.2930(3)	22.2967(3)	22.2915(3)
<i>c</i> (Å)	7.67969(11)	7.67933(10)	7.67609(10)	7.67808(11)
<i>V</i> (Å ³)	2082.83(6)	2082.02(5)	2081.26(5)	2081.08(5)
ρ_{calc} (g/cm ³)	5.75	5.748	5.745	5.741
ρ_{meas} (g/cm ³)	5.678	5.682	5.676	5.676
ρ_{rela} (%)	98.75	98.85	98.80	98.87

B(1)–O (Å)	1.9568(68)	1.9658(60)	1.9472(57)	1.9331(63)
B(2)–O (Å)	1.9521(68)	1.9514(65)	1.9417(66)	1.9428(69)
B(3)–O (Å)	1.9593(76)	1.9556(69)	1.9701(66)	1.9810(69)
B(4)–O (Å)	1.9906(71)	1.9941(63)	1.9902(63)	1.9782(68)
B(5)–O (Å)	1.9937(68)	1.9800(64)	1.9821(63)	1.9860(67)
A1(1)–O (Å)	2.6661(75)	2.6907(71)	2.6662(69)	2.6633(73)
A1(2)–O (Å)	2.7089(79)	2.7150(74)	2.7214(73)	2.7373(76)
A1(3)–O (Å)	2.7075(78)	2.6770(80)	2.7063(70)	2.6991(79)
A1(4)–O (Å)	2.7230(74)	2.7370(73)	2.7392(77)	2.7244(70)
A1(5)–O (Å)	2.6497(80)	2.6431(74)	2.6493(79)	2.6661(80)
A2(1)–O (Å)	3.1816(76)	3.1998(65)	3.1776(65)	3.1884(72)
A2(2)–O (Å)	3.1166(79)	3.1009(68)	3.1107(66)	3.0899(73)
avg(B–O) (Å)	1.9720(70)	1.9698(65)	1.9684(64)	1.9677(68)
avg(A1–O) (Å)	2.6910(77)	2.6926(74)	2.6965(74)	2.6980(76)
avg(A2–O) (Å)	3.1491(78)	3.1504(67)	3.1442(66)	3.1392(73)

Table S2 The structural parameters and reliability factors of the BNT–AN ceramics ($0.25 \leq z \leq 2$) obtained by

Rietveld refinement

<i>z</i>	<i>z</i> = 0.25	<i>z</i> = 0.5	<i>z</i> = 0.75	<i>z</i> = 1
<i>T</i> _{sinter} (°C)	1450	1450	1450	1400
<i>R</i> _p (%)	3.98	3.99	3.96	3.97
<i>R</i> _{wp} (%)	5.18	5.16	5.16	5.13

χ^2	2.6	2.56	2.47	2.32
a (Å)	12.18593(16)	12.18089(16)	12.17527(16)	12.17083(16)
b (Å)	22.3041(3)	22.3030(3)	22.2990(3)	22.2982(3)
c (Å)	7.68745(9)	7.68561(9)	7.68406(9)	7.68218(9)
V (Å ³)	2089.42(5)	2087.95(5)	2086.19(5)	2084.85(5)
ρ_{calc} (g/cm ³)	5.767	5.782	5.797	5.812
ρ_{meas} (g/cm ³)	5.687	5.711	5.716	5.721
ρ_{rela} (%)	98.61%	98.77%	98.60%	98.43%
B(1)–O (Å)	1.9422(55)	1.9520(52)	1.9366(51)	1.9386(49)
B(2)–O (Å)	1.9556(62)	1.9421(63)	1.9447(61)	1.9402(63)
B(3)–O (Å)	1.9493(64)	1.9523(66)	1.9651(63)	1.9693(64)
B(4)–O (Å)	1.9915(62)	2.0002(62)	1.9802(60)	1.9798(61)
B(5)–O (Å)	1.9928(63)	1.9886(63)	1.9943(62)	1.9964(64)
A1(1)–O (Å)	2.6799(65)	2.6941(63)	2.6839(65)	2.6990(65)
A1(2)–O (Å)	2.7265(66)	2.7181(62)	2.7138(63)	2.7106(66)
A1(3)–O (Å)	2.6977(67)	2.6752(72)	2.6947(65)	2.6961(71)
A1(4)–O (Å)	2.7184(64)	2.7193(64)	2.7215(64)	2.7097(65)
A1(5)–O (Å)	2.6685(71)	2.6768(74)	2.6702(69)	2.6794(71)
A2(1)–O (Å)	3.1702(65)	3.1801(68)	3.1443(59)	3.1502(62)
A2(2)–O (Å)	3.1315(64)	3.1279(68)	3.1602(59)	3.1349(63)
avg(B–O) (Å)	1.9690(62)	1.9687(62)	1.9672(60)	1.9678(61)
avg(A1–O) (Å)	2.6982(67)	2.6967(67)	2.6968(65)	2.6990(68)

avg(A2–O) (Å)	3.1509(65)	3.1540(68)	3.1523(59)	3.1426(63)
<i>z</i>	<i>z</i> = 1.25	<i>z</i> = 1.5	<i>z</i> = 1.75	<i>z</i> = 2
<i>T</i> _{sinter} (°C)	1400	1450	1500	1550
<i>R</i> _p (%)	3.9	3.75	3.86	3.84
<i>R</i> _{wp} (%)	5.08	4.9	5.06	4.97
χ^2	2.41	2.07	2.32	2.21
<i>a</i> (Å)	12.16521(16)	12.15803(16)	12.15348(16)	12.14878(17)
<i>b</i> (Å)	22.2980(3)	22.2928(3)	22.2927(3)	22.2923(3)
<i>c</i> (Å)	7.67938(9)	7.67813(9)	7.67588(9)	7.67412(10)
<i>V</i> (Å ³)	2083.11(5)	2081.06(5)	2079.66(5)	2078.34(5)
ρ_{calc} (g/cm ³)	5.828	5.844	5.859	5.874
ρ_{meas} (g/cm ³)	5.711	5.711	5.725	5.649
ρ_{rela} (%)	97.99%	97.72%	97.71%	96.17%
B(1)–O (Å)	1.9342(49)	1.9480(49)	1.9410(51)	1.9562(47)
B(2)–O (Å)	1.9397(60)	1.9347(60)	1.9339(60)	1.9278(60)
B(3)–O (Å)	1.9675(62)	1.9664(62)	1.9721(61)	1.9705(62)
B(4)–O (Å)	1.9884(59)	1.9952(59)	1.9826(59)	1.9836(59)
B(5)–O (Å)	1.9850(62)	1.9911(62)	1.9952(61)	1.9969(62)
A1(1)–O (Å)	2.6926(63)	2.6828(62)	2.6816(63)	2.6932(60)
A1(2)–O (Å)	2.7047(63)	2.7148(61)	2.7089(61)	2.7071(58)
A1(3)–O (Å)	2.6846(63)	2.6786(65)	2.6755(65)	2.6787(64)

A1(4)–O (Å)	2.7164(63)	2.7081(63)	2.7073(64)	2.7132(66)
A1(5)–O (Å)	2.6813(69)	2.6794(66)	2.6871(68)	2.6866(69)
A2(1)–O (Å)	3.1451(61)	3.1344(59)	3.1271(60)	3.1197(61)
A2(2)–O (Å)	3.1572(61)	3.1603(60)	3.1714(61)	3.1623(61)
avg(B–O) (Å)	1.9662(59)	1.9692(59)	1.9676(59)	1.9682(59)
avg(A1–O) (Å)	2.6959(64)	2.6927(63)	2.6921(64)	2.6958(63)
avg(A2–O) (Å)	3.1512(61)	3.1474(60)	3.1493(61)	3.1410(61)

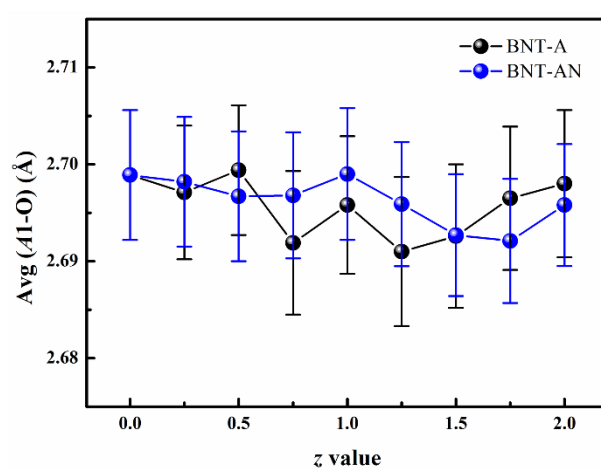


Fig. S1 The average bond length of A1–O in the BNT–A and BNT–AN ($0 \leq z \leq 2$) ceramics.