**Supplementary Material**

Table S1. The structural parameters and reliability factors of the BNT-A ceramics (0 ≤ z ≤ 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* (Å3) | 2091.19(5) | 2089.03(5) | 2087.52(5) | 2085.82(5) | 2084.19(5) |
| *ρ*calc (g/cm3) | 5.751 | 5.752 | 5.752 | 5.752 | 5.751 |
| *ρ*meas (g/cm3) | 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) |
| *A*1(1)-O (Å) | 2.6899(63) | 2.6679(68) | 2.6855(64) | 2.6624(72) | 2.6623(66) |
| *A*1(2)-O (Å) | 2.7172(65) | 2.7241(68) | 2.7114(65) | 2.7187(75) | 2.7258(69) |
| *A*1(3)-O (Å) | 2.6954(67) | 2.7037(69) | 2.7070(67) | 2.6978(73) | 2.7001(73) |
| *A*1(4)-O (Å) | 2.7235(68) | 2.7069(68) | 2.7198(67) | 2.7351(73) | 2.7349(71) |
| *A*1(5)-O (Å) | 2.6684(73) | 2.6827(73) | 2.6733(71) | 2.6454(76) | 2.6558(76) |
| *A*2(1)-O (Å) | 3.1568(62) | 3.1542(62) | 3.1570(64) | 3.1902(71) | 3.2007(66) |
| *A*2(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(*A*1-O) (Å) | 2.6989(67) | 2.6971(69) | 2.6994(67) | 2.6919(74) | 2.6958(71) |
| avg(*A*2-O) (Å) | 3.1501(63) | 3.1521(62) | 3.1476(64) | 3.1583(72) | 3.1474(67) |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *z* | *z* = 1.25 | *z* = 1.5 | *z* = 1.75 | *z* = 2 |
| *T*sinter (°C) | 1400 | 1350 | 1350 | 1400 |
| *R*p (%) | 4.47 | 4.30 | 4.26 | 4.30 |
| *R*wp (%) | 6.24 | 5.81 | 5.72 | 5.74 |
| *χ*2 | 3.44 | 3.05 | 3.37 | 3.26 |
| *a* (Å) | 12.16431(19) | 12.16168(18) | 12.16032(18) | 12.15894(19) |
| *b* (Å) | 22.2957(4) | 22.2930(3) | 22.2967(3) | 22.2915(3) |
| *c* (Å) | 7.67969(11) | 7.67933(10) | 7.67609(10) | 7.67808(11) |
| *V* (Å3) | 2082.83(6) | 2082.02(5) | 2081.26(5) | 2081.08(5) |
| *ρ*calc (g/cm3) | 5.75 | 5.748 | 5.745 | 5.741 |
| *ρ*meas (g/cm3) | 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) |
| *A*1(1)-O (Å) | 2.6661(75) | 2.6907(71) | 2.6662(69) | 2.6633(73) |
| *A*1(2)-O (Å) | 2.7089(79) | 2.7150(74) | 2.7214(73) | 2.7373(76) |
| *A*1(3)-O (Å) | 2.7075(78) | 2.6770(80) | 2.7063(70) | 2.6991(79) |
| *A*1(4)-O (Å) | 2.7230(74) | 2.7370(73) | 2.7392(77) | 2.7244(70) |
| *A*1(5)-O (Å) | 2.6497(80) | 2.6431(74) | 2.6493(79) | 2.6661(80) |
| *A*2(1)-O (Å) | 3.1816(76) | 3.1998(65) | 3.1776(65) | 3.1884(72) |
| *A*2(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(*A*1-O) (Å) | 2.6910(77) | 2.6926(74) | 2.6965(74) | 2.6980(76) |
| avg(*A*2-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 ≤ z ≤ 2) obtained by Rietveld refinement.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *z* | *z* = 0.25 | *z* = 0.5 | *z* = 0.75 | *z* = 1 |
| *T*sinter (°C) | 1450 | 1450 | 1450 | 1400 |
| *R*p (%) | 3.98 | 3.99 | 3.96 | 3.97 |
| *R*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* (Å3) | 2089.42(5) | 2087.95(5) | 2086.19(5) | 2084.85(5) |
| *ρ*calc (g/cm3) | 5.767 | 5.782 | 5.797 | 5.812 |
| *ρ*meas (g/cm3) | 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) |
| *A*1(1)-O (Å) | 2.6799(65) | 2.6941(63) | 2.6839(65) | 2.6990(65) |
| *A*1(2)-O (Å) | 2.7265(66) | 2.7181(62) | 2.7138(63) | 2.7106(66) |
| *A*1(3)-O (Å) | 2.6977(67) | 2.6752(72) | 2.6947(65) | 2.6961(71) |
| *A*1(4)-O (Å) | 2.7184(64) | 2.7193(64) | 2.7215(64) | 2.7097(65) |
| *A*1(5)-O (Å) | 2.6685(71) | 2.6768(74) | 2.6702(69) | 2.6794(71) |
| *A*2(1)-O (Å) | 3.1702(65) | 3.1801(68) | 3.1443(59) | 3.1502(62) |
| *A*2(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(*A*1-O) (Å) | 2.6982(67) | 2.6967(67) | 2.6968(65) | 2.6990(68) |
| avg(*A*2-O) (Å) | 3.1509(65) | 3.1540(68) | 3.1523(59) | 3.1426(63) |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *z* | *z* = 1.25 | *z* = 1.5 | *z* = 1.75 | *z* = 2 |
| *T*sinter (°C) | 1400 | 1450 | 1500 | 1550 |
| *R*p (%) | 3.9 | 3.75 | 3.86 | 3.84 |
| *R*wp (%) | 5.08 | 4.9 | 5.06 | 4.97 |
| *χ*2 | 2.41 | 2.07 | 2.32 | 2.21 |
| *a* (Å) | 12.16521(16) | 12.15803(16) | 12.15348(16) | 12.14878(17) |
| *b* (Å) | 22.2980(3) | 22.2928(3) | 22.2927(3) | 22.2923(3) |
| *c* (Å) | 7.67938(9) | 7.67813(9) | 7.67588(9) | 7.67412(10) |
| *V* (Å3) | 2083.11(5) | 2081.06(5) | 2079.66(5) | 2078.34(5) |
| *ρ*calc (g/cm3) | 5.828 | 5.844 | 5.859 | 5.874 |
| *ρ*meas (g/cm3) | 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) |
| *A*1(1)-O (Å) | 2.6926(63) | 2.6828(62) | 2.6816(63) | 2.6932(60) |
| *A*1(2)-O (Å) | 2.7047(63) | 2.7148(61) | 2.7089(61) | 2.7071(58) |
| *A*1(3)-O (Å) | 2.6846(63) | 2.6786(65) | 2.6755(65) | 2.6787(64) |
| *A*1(4)-O (Å) | 2.7164(63) | 2.7081(63) | 2.7073(64) | 2.7132(66) |
| *A*1(5)-O (Å) | 2.6813(69) | 2.6794(66) | 2.6871(68) | 2.6866(69) |
| *A*2(1)-O (Å) | 3.1451(61) | 3.1344(59) | 3.1271(60) | 3.1197(61) |
| *A*2(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(*A*1-O) (Å) | 2.6959(64) | 2.6927(63) | 2.6921(64) | 2.6958(63) |
| avg(*A*2-O) (Å) | 3.1512(61) | 3.1474(60) | 3.1493(61) | 3.1410(61) |



Fig. S1 The average bond length of *A*1-O in the BNT-A and BNT-AN (0 ≤ *z* ≤ 2) ceramics.