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Nanoscale

Supplementary Information

Precursor Effects and Formation Mechanism of Polyol-Synthesized Thermoelectric Bi_2Te_3

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Themed Collection: *Thermoelectric Energy Conversion*

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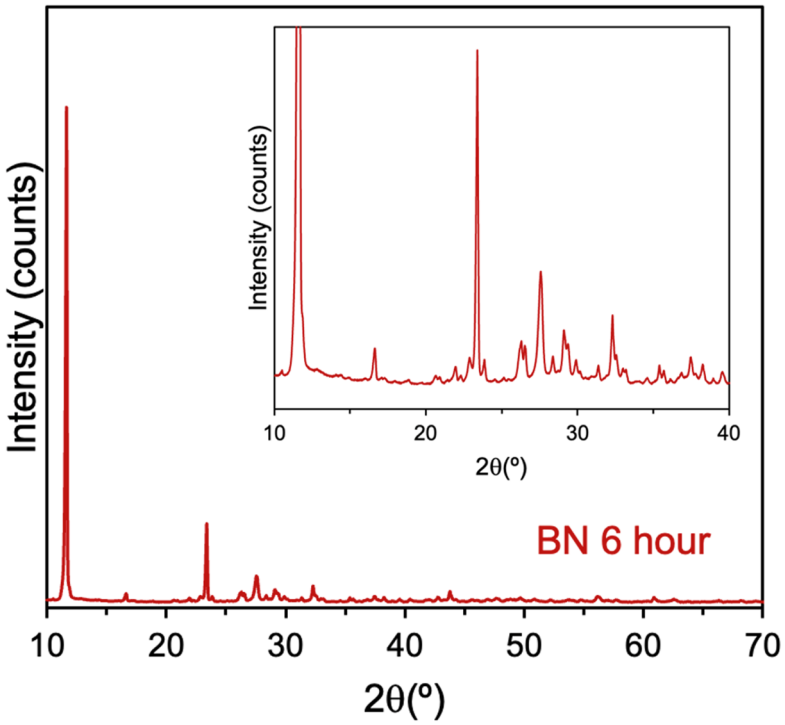

Figure S1. PXRD Pattern from 10º–70º and magnified from 10º–40º for $Bi_3(C_2H_4O_2)_4NO_3$ (6-hour aliquot).

Table S1. Atomic coordinates and equivalent isotropic displacement parameters for $Bi_3(C_2H_4O_2)_4NO_3$.

Atom	Wyckoff Position	*x*	*y*	*z*	*U* (Å^2)
Bi(1)	4e	0.7179(1)	0.2010(1)	0.1973(1)	0.014(1)
Bi(2)	4e	0.9667(1)	0.2399(1)	0.4513(1)	0.015(1)
Bi(3)	4e	0.2173(1)	0.2872(1)	0.2055(1)	0.014(1)
C(1)	4e	0.7169(9)	0.3954(4)	0.4409(4)	0.021(1)
C(2)	4e	0.6294(8)	0.3424(4)	0.3590(4)	0.021(1)
C(3)	4e	0.1325(8)	0.1032(4)	0.2762(5)	0.026(1)
C(4)	4e	0.3278(9)	0.1178(4)	0.3111(5)	0.029(2)
C(5)	4e	0.2975(8)	0.1487(4)	0.0350(4)	0.021(1)
C(6)	4e	0.2096(8)	0.1032(4)	-0.0527(4)	0.019(1)
C(7)	4e	0.7971(8)	0.3848(4)	0.1234(4)	0.021(1)
C(8)	4e	0.6060(8)	0.3674(4)	0.0866(4)	0.024(1)
H(1A)	4e	0.8050	0.4349	0.4153	0.025
H(1B)	4e	0.6268	0.4306	0.4712	0.025
H(2A)	4e	0.5261	0.3111	0.3814	0.025
H(2B)	4e	0.5893	0.3810	0.3061	0.025
H(3A)	4e	0.1278	0.0746	0.2131	0.032
H(3B)	4e	0.0739	0.0653	0.3215	0.032
H(4A)	4e	0.3333	0.1343	0.3792	0.035
H(4B)	4e	0.3948	0.0636	0.3046	0.035
H(5A)	4e	0.3294	0.1059	0.0852	0.026
H(5B)	4e	0.4060	0.1784	0.0171	0.026
H(6A)	4e	0.2980	0.0683	-0.0845	0.022
H(6B)	4e	0.1161	0.0640	-0.0322	0.022
H(7A)	4e	0.8557	0.4231	0.0785	0.026
H(7B)	4e	0.7978	0.4137	0.1862	0.026
H(8A)	4e	0.5358	0.4209	0.0905	0.029
H(8B)	4e	0.6042	0.3490	0.0192	0.029
O(1)	4e	0.8018(6)	0.3391(3)	0.5113(3)	0.022(1)
O(2)	4e	0.7585(5)	0.2818(3)	0.3265(3)	0.018(1)
O(3)	4e	0.0418(5)	0.1856(3)	0.2693(3)	0.017(1)
O(4)	4e	0.4055(5)	0.1849(3)	0.2558(3)	0.019(1)
O(5)	4e	0.1743(5)	0.2103(3)	0.0699(3)	0.021(1)
O(6)	4e	0.1344(6)	0.1668(3)	-0.1185(2)	0.022(1)
O(7)	4e	0.8919(5)	0.3028(3)	0.1321(3)	0.017(1)
O(8)	4e	0.5296(5)	0.3002(3)	0.1441(3)	0.019(1)
O(9)	4e	0.2929(9)	0.4837(4)	0.2343(3)	0.056(2)
O(10)	4e	0.2576(7)	0.5895(3)	0.1318(3)	0.036(1)
O(11)	4e	0.2017(7)	0.4547(4)	0.0870(4)	0.044(1)
N(1)	4e	0.2499(7)	0.5091(4)	0.1506(4)	0.028(1)

Table S2. Bond lengths for $Bi_3(C_2H_4O_2)_4NO_3$.

Atom Pair	Distance (Å)	Atom Pair	Distance (Å)
Bi(1)-O(1)	2.737(4)	C(3)-H(3B)	0.97
Bi(1)-O(2)	2.171(4)	C(4)-H(4A)	0.97
Bi(1)-O(3)	2.576(4)	C(4)-H(4B)	0.97
Bi(1)-O(4)	2.516(4)	C(5)-C(6)	1.513(8)
Bi(1)-O(7)	2.237(4)	C(5)-H(5A)	0.97
Bi(1)-O(8)	2.164(4)	C(5)-H(5B)	0.97
Bi(2)-O(1)	2.139(4)	C(6)-H(6A)	0.97
Bi(2)-O(2)	2.346(4)	C(6)-H(6B)	0.97
Bi(2)-O(3)	2.725(4)	C(7)-C(8)	1.512(8)
Bi(2)-O(5)	2.320(4)	C(7)-H(7A)	0.97
Bi(2)-O(6)	2.150(4)	C(7)-H(7B)	0.97
Bi(2)-O(7)	2.659(4)	C(8)-H(8A)	0.97
Bi(3)-O(3)	2.233(4)	C(8)-H(8B)	0.97
Bi(3)-O(4)	2.184(4)	O(1)-C(1)	1.418(7)
Bi(3)-O(5)	2.214(4)	O(2)-C(2)	1.421(7)
Bi(3)-O(6)	2.626(4)	O(3)-C(3)	1.424(7)
Bi(3)-O(7)	2.594(4)	O(4)-C(4)	1.415(7)
Bi(3)-O(8)	2.526(4)	O(5)-C(5)	1.413(7)
C(1)-C(2)	1.507(8)	O(6)-C(6)	1.421(6)
C(1)-H(1A)	0.97	O(7)-C(7)	1.434(7)
C(1)-H(1B)	0.97	O(8)-C(8)	1.428(7)
C(2)-H(2A)	0.97	N(1)-O(9)	1.242(7)
C(2)-H(2B)	0.97	N(1)-O(11)	1.244(7)
C(3)-C(4)	1.527(9)	N(1)-O(10)	1.250(7)
C(3)-H(3A)	0.97		

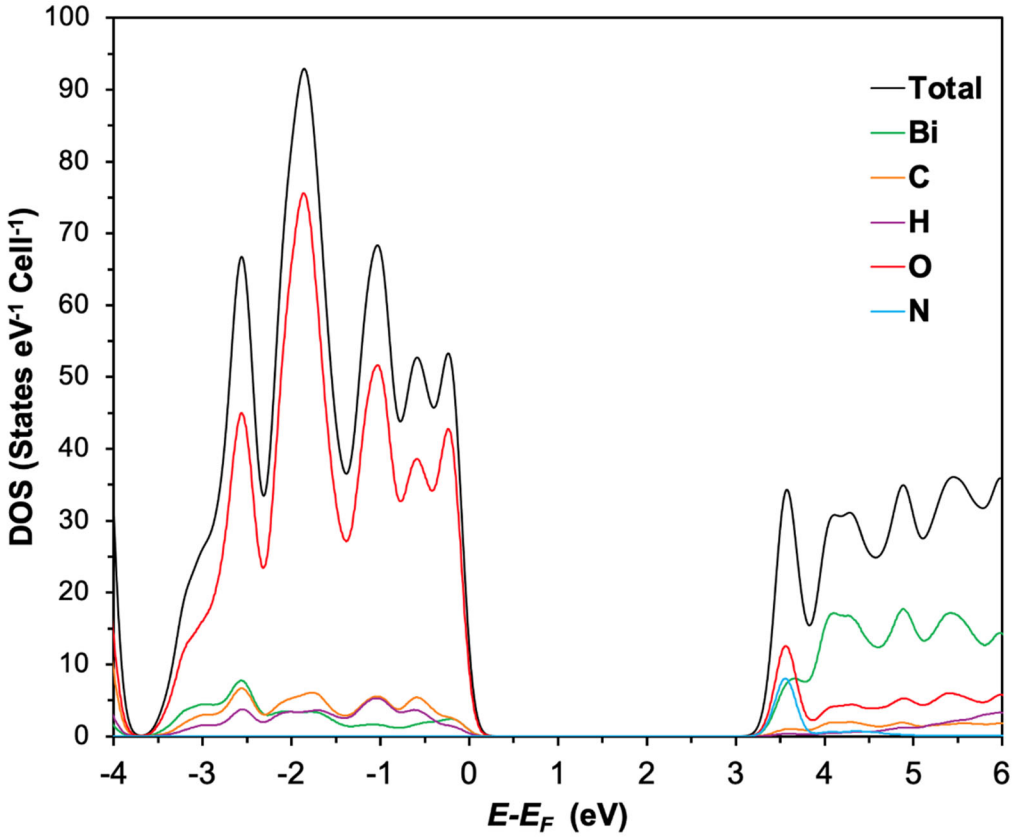

Figure S2. Density Of States (DOS) of $Bi_3(C_2H_4O_2)_4NO_3$.

Table S3. Diameter and thickness of hot-pressed Bi_2Te_3 pellets from Bi_2O_3 (BO) and $Bi(NO_3)_3 \cdot 5H_2O$ (BN).

Sample	Diameter	Thickness
Bi_2Te_3 from Bi_2O_3 (BO)	12.7 mm	6.57 mm
Bi_2Te_3 from $Bi(NO_3)_3 \cdot 5H_2O$ (BN)	12.7 mm	6.40 mm

Table S4. PXRD unit cell refinement results for BO and BN in hot-pressed pellet form.

Sample	*a* (Å)	*c* (Å)	*V* (Å^3)
Hot-pressed BO pellet	4.38029(2)	30.4174(1)	505.43(4)
Hot-pressed BN pellet	4.37983(2)	30.4697(6)	506.19(4)

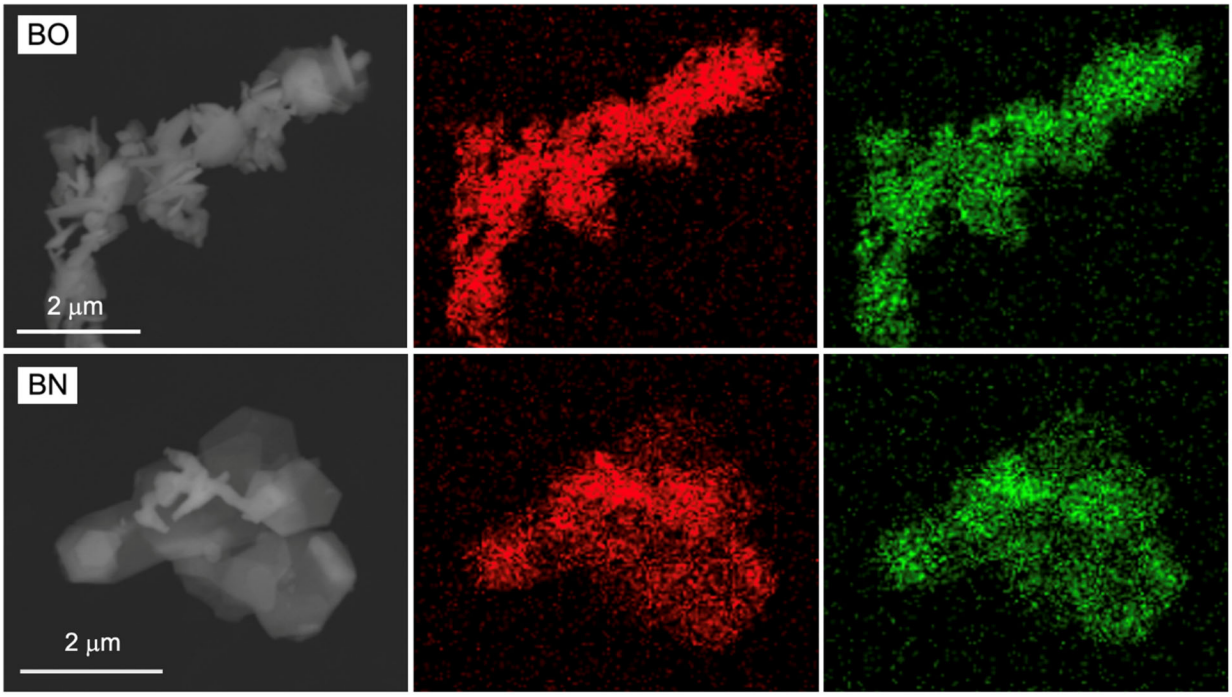

Figure S3. SEM-EDS maps for BO and BN with Bi in red and Te in green.

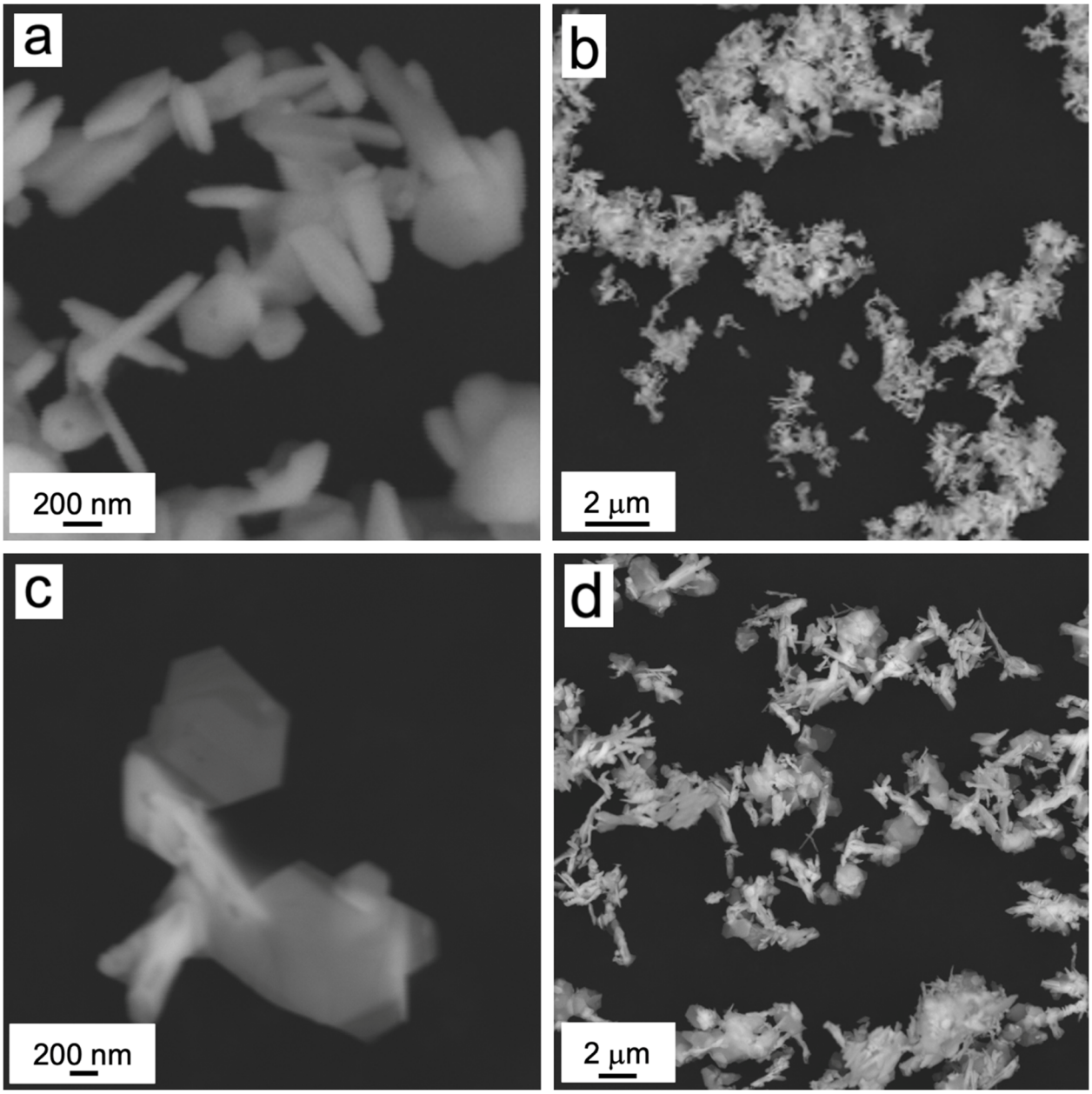

Figure S4. SEM images for a) BO at 200 nm, b) BO at 2 μm, c) BN at 200 nm, and d) BN at 2 μm.

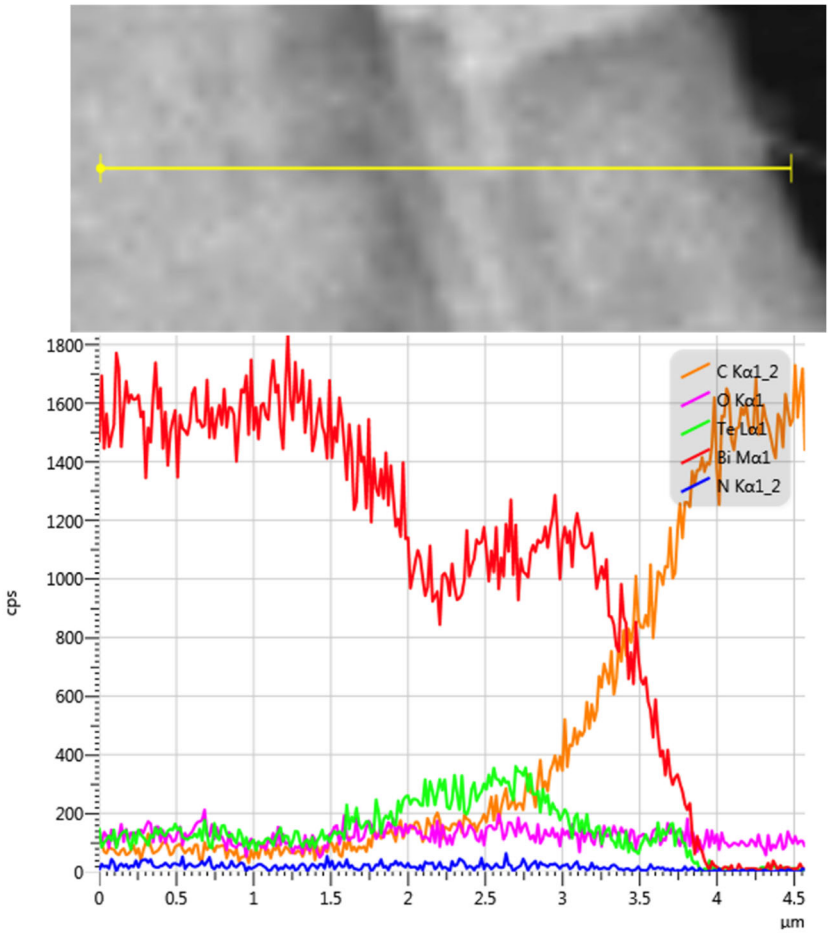

Figure S5. SEM-EDS line image and plot for BN after 9 hours.

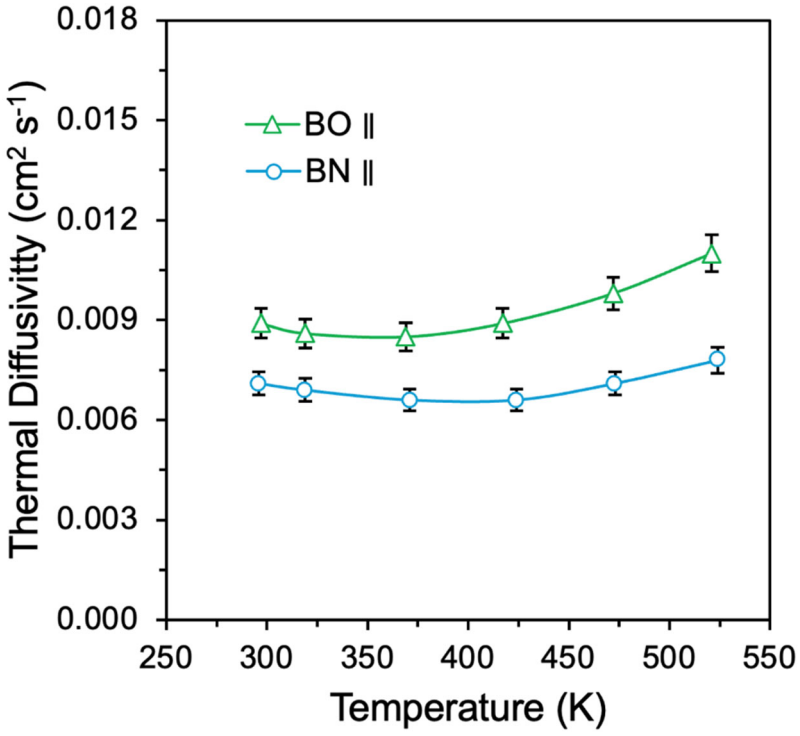

Figure S6. Temperature dependence of thermal diffusivity for BO (‖) and BN (‖).