— Supplementary Information —

Mechanochemical Synthesis of Ba-Doped BiCuSeO Oxyselenides: Influence of Processing Conditions on Phase Formation

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Phase and elemental analysis

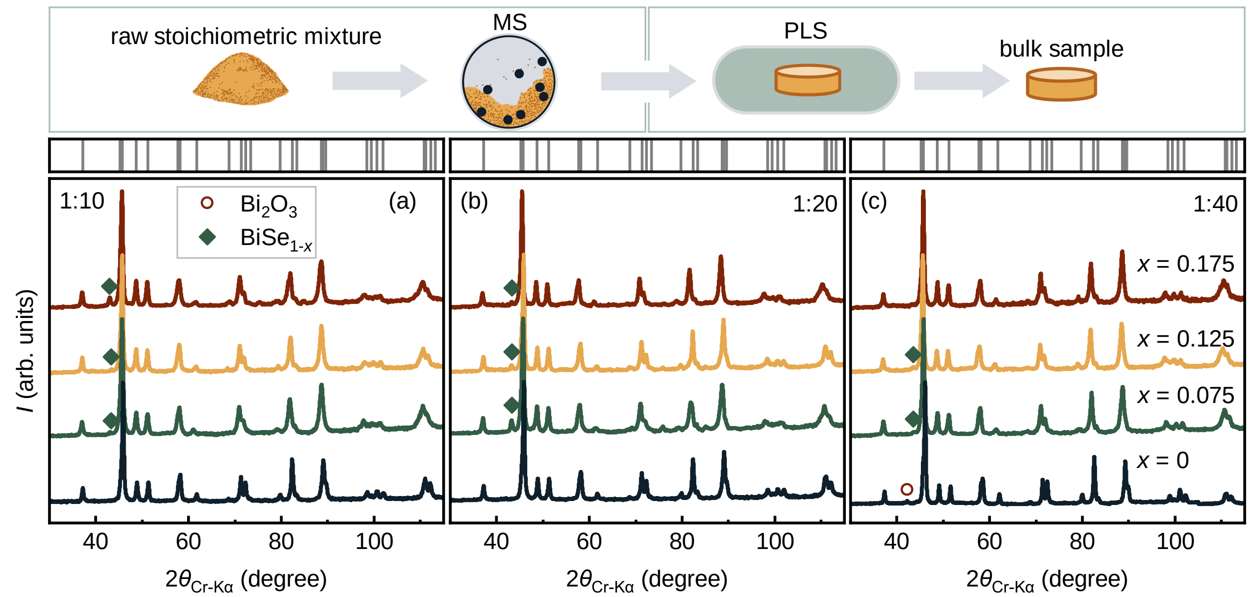

Figure S1: Powder XRD patterns of the $Bi_{1-x}Ba_xCuSeO$ (x = 0, 0.075, 0.125, 0.175) samples after MS and PLS. Bragg's reflections for the BiCuSeO phase are indicated by gray ticks on the top part of the figure.

Table S1: Refined lattice constants from Rietveld analysis of X-ray diffraction data and EDS results for the $Bi_{1-x}Ba_xCuSeO$ (x = 0, 0.075, 0.125, 0.175) samples grounded in different powder-to-ball mass ratios after MS

powder-to-ball mass ratio	Nominal composition	a, b (Å)	c (Å)	(Bi + Ba):Cu:Se ratios	Ba/(Bi + Ba)	d_{CS} (Å)
1:10	BiCuSeO	3.929	8.931	1.08:0.86:1.05	0	201
	$Bi_{0.925}Ba_{0.075}CuSeO$	3.946	9.013	1.05:0.93:1.02	0.07	344
	$Bi_{0.875}Ba_{0.125}CuSeO$	3.953	9.041	1.04:0.96:1.01	0.12	269
	$Bi_{0.825}Ba_{0.175}CuSeO$	3.959	9.074	1.03:0.99:0.98	0.16	256
1:20	BiCuSeO	3.928	8.948	1.02:0.94:0.99	0	250
	$Bi_{0.925}Ba_{0.075}CuSeO$	3.939	8.992	1.01:0.99:0.98	0.07	219
	$Bi_{0.875}Ba_{0.125}CuSeO$	3.947	9.030	1.02:0.99:0.99	0.12	209
	$Bi_{0.825}Ba_{0.175}CuSeO$	3.954	9.064	1.01:0.99:0.99	0.16	225
1:40	BiCuSeO	3.926	8.950	1.03:0.99:0.98	0	225
	$Bi_{0.925}Ba_{0.075}CuSeO$	3.943	9.000	1.02:0.99:0.99	0.07	213
	$Bi_{0.875}Ba_{0.125}CuSeO$	3.950	9.041	1.02:1.00:0.98	0.11	196
	$Bi_{0.825}Ba_{0.175}CuSeO$	3.957	9.075	1.02:1.00:0.99	0.17	210

Particle size distribution

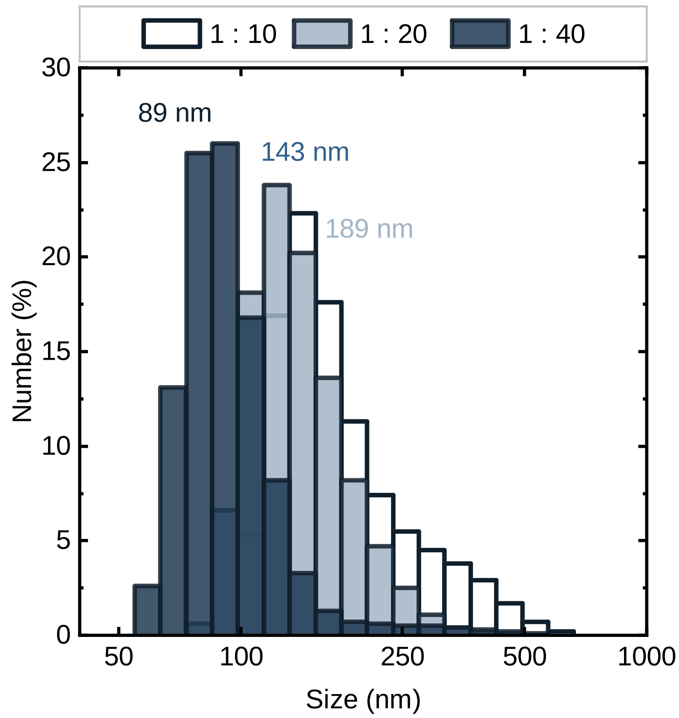

Figure S2: Particle size distribution of BiCuSeO powders milled at different powder-to-ball mass ratios.

Microstructure characterization

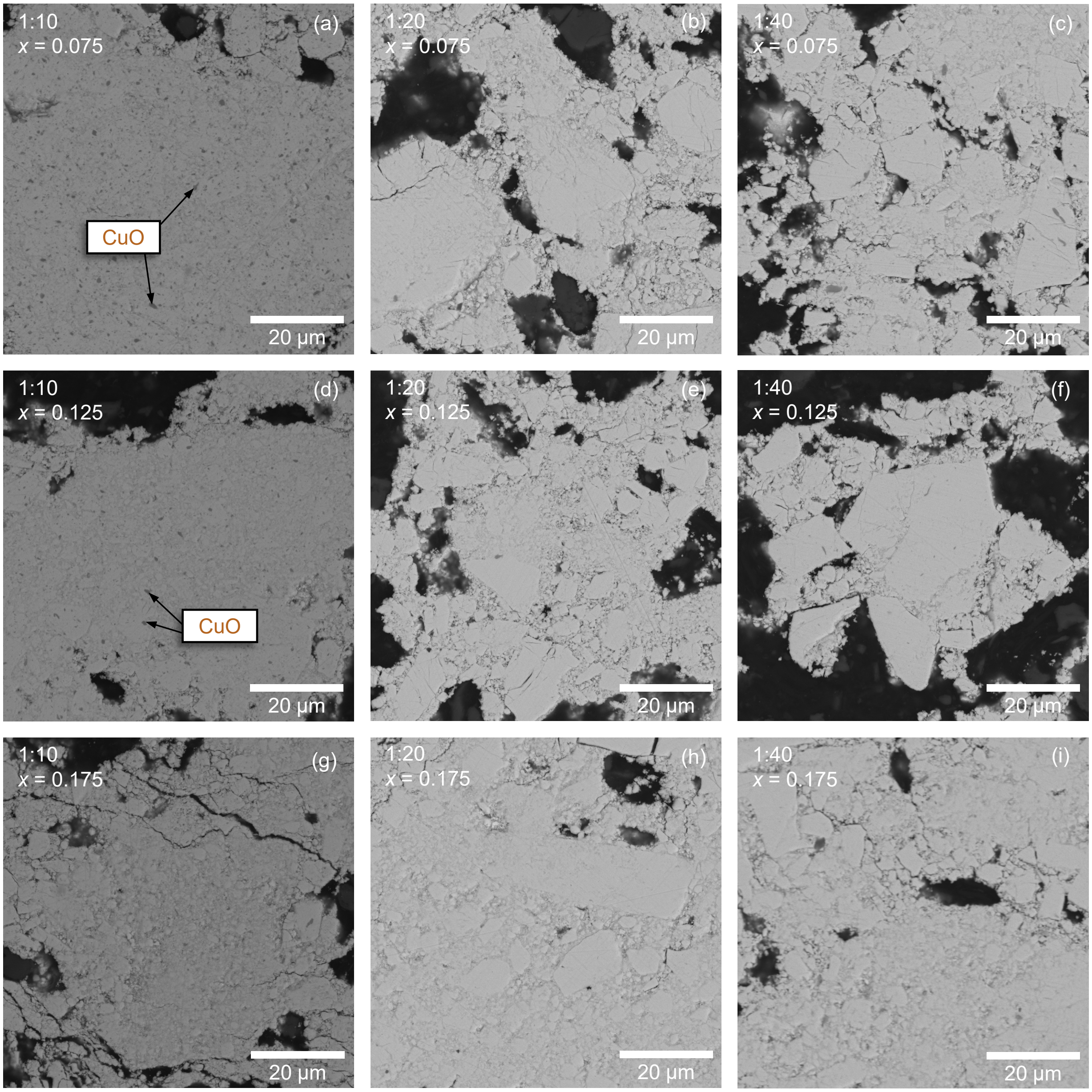

Figure S3: SEM micrographs of the polished surfaces for $Bi_{1-x}Ba_xCuSeO$ ($x = 0.075$, 0.125, 0.175) powders. The dark areas are CuO phases.

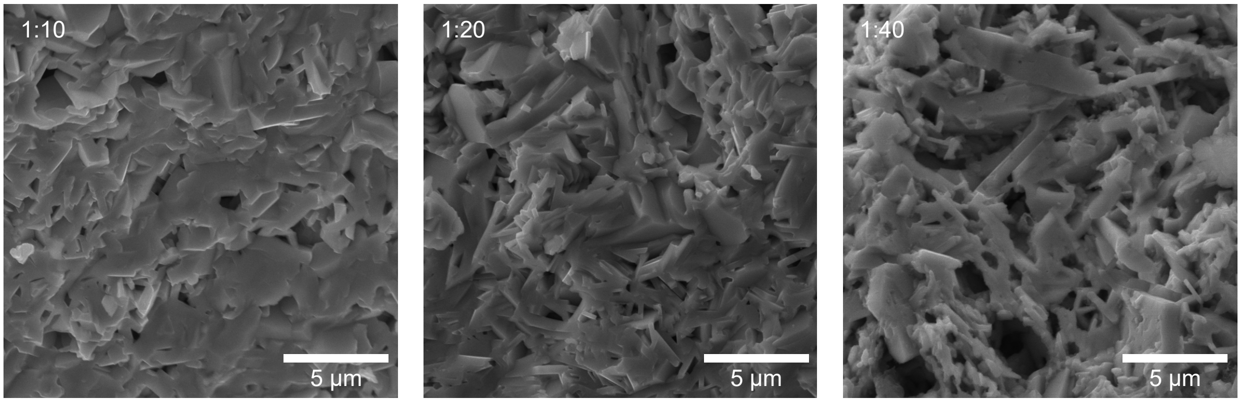

Figure S4: SEM micrographs of the fractured cross-sections for BiCuSeO bulk samples.

Thermal conductivity and figure of merit

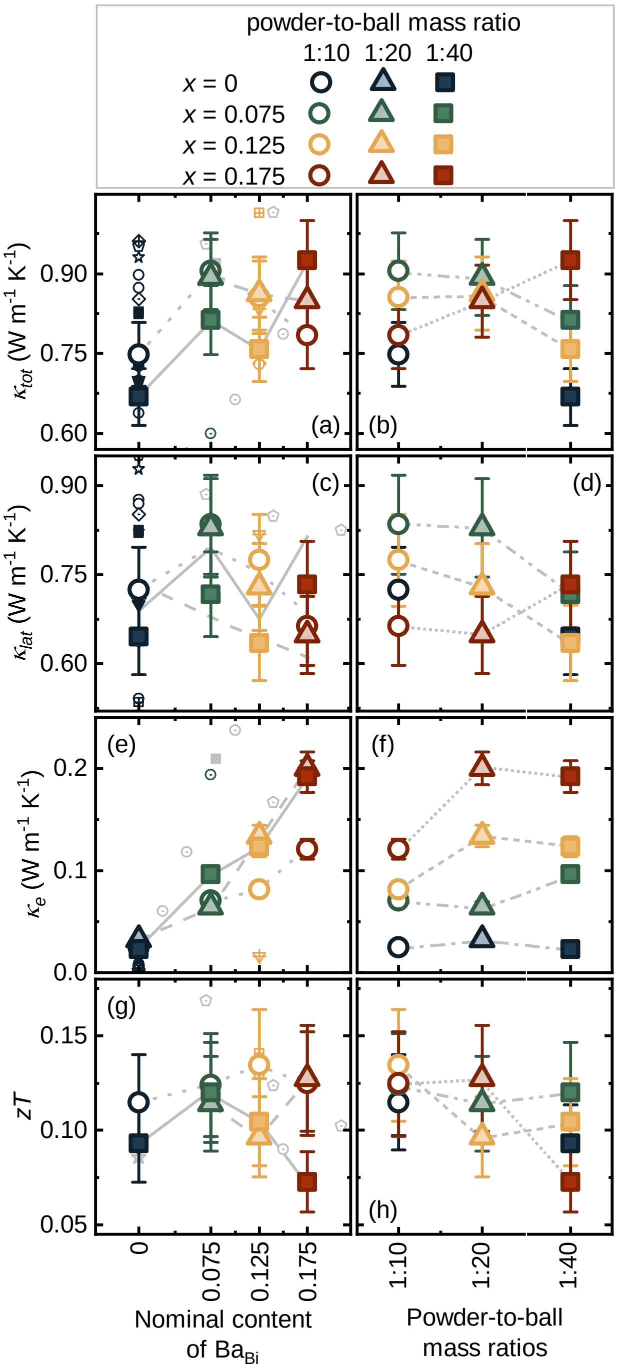

Figure S5: Concentration and powder-to-ball mass ratio dependence of the (a, b) total thermal conductivity κ_{tot}, (c, d) lattice thermal conductivity κ_{lat} and (e, f) electrical thermal conductivity κ_{el} and (g, h) figure of merit zT for $Bi_{1-x}Ba_xCuSeO$ (x = 0, 0.075, 0.125, 0.175) samples consolidated by PLS. Literature data for other $Bi_{1-x}Ba_xCuSeO$-based oxyselenides are also shown for comparison (Bhaskar et al.,[1] Feng et al.,[2,3] Hong et al.,[4] Lan et al.,[5] Liu et al.,[6] Jiang et al.,[7] Kim et al.,[8] Lei et al.,[9,10] Li et al.,[11,12] Liang et al.,[13] Park et al.,[14] Luu et al.,[15] Pei et al.,[16] Novitskii et al,[17] Wen et al.,[18] Yang et al.,[19] Zeng et al.[20]). All displayed data points correspond to values obtained at 300 K.

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