Electronic Supplementary Material (ESI) for Nanoscale.
This journal is © The Royal Society of Chemistry 2018

Supporting Information for

Optimizing Interfacial Transport Properties of InO_2 Single Atomic Layers in $In_2O_3(ZnO)_4$ Natural Superlattices for Enhanced High Temperature Thermoelectrics

Xin Liang* and Lei Shen

School of Materials Science and Engineering, Changzhou University, Changzhou, Jiangsu 213164, China

*Corresponding author (X. Liang): liangxin@cczu.edu.cn

Table SI. Ionic size difference of Al^{3+} and Ce^{4+} with respect to Zn^{2+} and In^{3+} ions. A positive value suggests a larger size of dopant ions (Al^{3+} or Ce^{4+}) over the host ones (Zn^{2+} or In^{3+}), and vice versa for a negative value.

	Ionic size difference (pm)	
	Zn^{2+}	In^{3+}
Al^{3+}	-23	-30
Ce^{4+}	+18	+11

Table SII. Nominal and actual doping concentration of Al and/or Ce in the $In_2O_3(ZnO)_4$ superlattices. The values of Zn and In concentration, [Zn] and [In], comes from the chemical formula of pristine $In_2O_3(ZnO)_4$.

	Nominal doping concentration, [Al]/([Zn]+[Al]) or [Ce]/([In]+[Ce])	Actual doping concentration, [Al]/([Zn]+[In]+[Al]) or [Ce]/([Zn]+[In]+[Ce])
Al doping	0.4 mol. %	0.27 mol. %
	0.8 mol. %	0.54 mol. %
	0.12 mol. %	0.80 mol. %
	0.16 mol. %	1.07 mol. %
	0.20 mol. %	1.34 mol. %
Ce doping	0.1 mol. %	0.033 mol. %
	0.2 mol. %	0.066 mol. %
	0.3 mol. %	0.099 mol. %
Al & Ce dual doping	0.4 mol. % Al & 0.2 mol. % Ce	0.27 mol. % Al, 0.066 mol. % Ce
	0.8 mol. % Al & 0.1 mol. % Ce	0.54 mol. % Al, 0.033 mol. % Ce
	1.0 mol. % Al & 0.2 mol. % Ce	0.67 mol. % Al, 0.066 mol. % Ce
	1.6 mol. % Al & 0.05 mol. % Ce	1.07 mol. % Al, 0.017 mol. % Ce
	1.6 mol. % Al & 0.2 mol. % Ce	1.07 mol. % Al, 0.066 mol. % Ce

Table SIII. Mass density, relative density and porosity of superlattice samples in the present work measured by Archimedes method. The relative density is calculated based on the theoretical mass density of the pristine $In_2O_3(ZnO)_4$ superlattice (6.19 g cm^{-3}).

Superlattice compositions	Mass density (g cm^{-3})	Relative density (%)	Porosity (%)
Pristine	5.63	90.95	9.05
0.4 mol. % Al	5.48	88.53	11.47
0.8 mol. % Al	5.45	88.05	11.95
1.2 mol. % Al	5.42	87.65	12.35
1.6 mol. % Al	5.51	89.01	10.99
2.0 mol. % Al	5.56	89.82	10.18
0.1 mol. % Ce	5.51	89.01	10.99
0.2 mol. % Ce	5.52	89.18	10.82
0.3 mol. % Ce	5.55	89.66	10.34
0.4 mol. % Al & 0.2 mol. % Ce	5.46	88.21	11.79
0.8 mol. % Al & 0.1 mol. % Ce	5.53	89.34	10.66
1.0 mol. % Al & 0.2 mol. % Ce	5.49	88.69	11.31
1.6 mol. % Al & 0.05 mol. % Ce	5.46	88.21	11.79
1.6 mol. % Al & 0.2 mol. % Ce	5.53	89.34	10.66

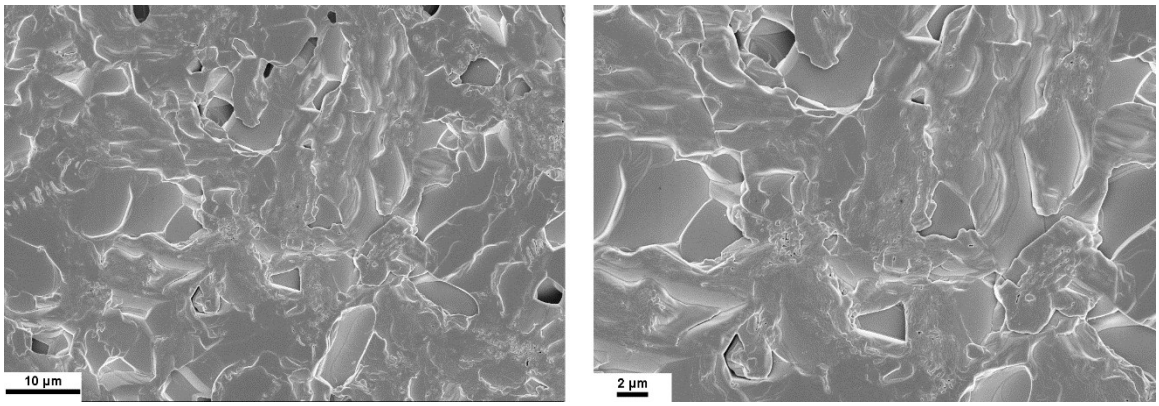

Figure S1. SEM image of the pristine $In_2O_3(ZnO)_4$ superlattice sample showing the typical grain size is about several micrometers.

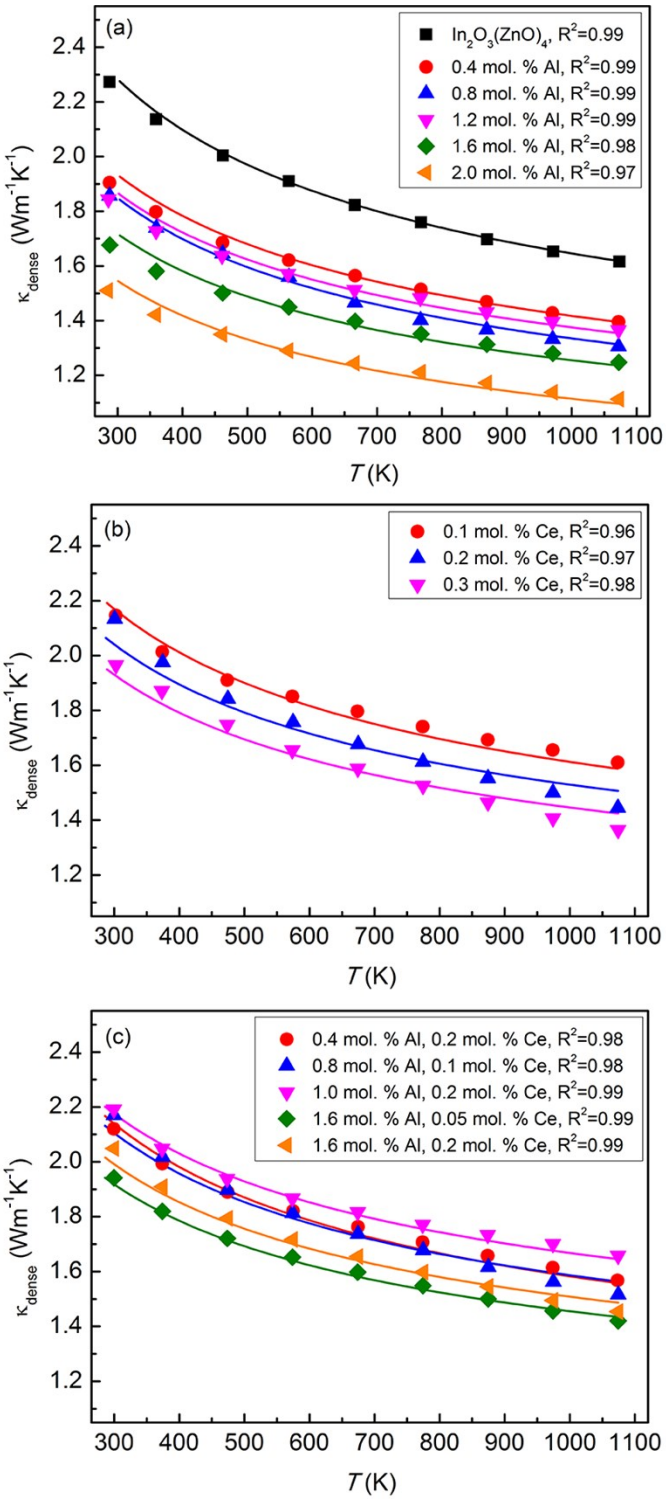

Figure S2. Fitting of measured temperature dependence of thermal conductivity (with porosity correction) by Klemens-Callaway model with correlational approximation, equation (6)-(8). The scattered data are measured values and solid curves are the best fit

with R^2 values indicated in the legend. (a) Al doping; (b) Ce doping; (c) Al and Ce dual doping.