Atomic-Level Control of the Thermoelectric Properties in Polytypoid Nanowires

Sean C. Andrews^{1,2}*, Melissa A. Fardy^{1,2}*, Michael C. Moore^{1,2}*, Shaul Aloni², Minjuan Zhang³, Velimir Radmilovic^{2,4}, & Peidong Yang^{1,2}

Instrumentation

SEM images were collected using a JEOL JSM 6340F field-emission SEM operating at 5 kV. XRD patterns were collected using a Bruker D8 GADDS diffractometer with Co k_{α} irradiation and a Bruker D8 Advance diffractometer with Cu k_{α} irradiation. Individual nanowires were imaged using the following: a Tecnai G2 S-Twin TEM operating at 200 kV, a Technai F20 UT TEM operating at 200 kV, a Philips CM200/FEG TEM operating at 200 kV and a JEOL JEM-2100 LaB₆ TEM operating at 200 kV. Elemental analysis was performed on a Hitachi H-7650 TEM operating at 120 kV equipped with an EDAX EDS. Elemental maps were collected using a JEOL JEM-2100-F field emission analytical TEM operating at 200 kV with a HAADF STEM detector and an Oxford EDS. The Z-contrast STEM images were taken using the transmission electron aberration-corrected microscope (TEAM) 0.5, which consists of a modified

¹Department of Chemistry, University of California, Berkeley, California 94720.

²Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720.

³Materials Research Department, Toyota Research Institute of North America, Toyota Motor Engineering & Manufacturing North America (TEMA) Inc., 1555 Woodridge Avenue, Ann Arbor, Michigan 48105

⁴National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, California 94720.

^{*}These authors contributed equally to this work.

FEI Titan 80-300 microscope equipped with a special high-brightness Schottky-field emission electron source, a gun monochromator, a high-resolution GIF Tridiem energy-filter, and two CEOS hexapole-type spherical aberration correctors, all of which enable 50 pm resolution. The TEAM 0.5 has a HAADF STEM detector and was operated at 300 kV.

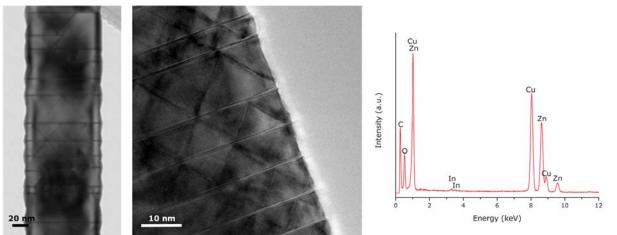


Figure S1: Indium zinc oxide (IZO) nanowires. TEM images and EDS spectrum of IZO nanowires prepared by coating ZnO nanowires with 15 nm of In and annealing at 1173 K in oxygen for 12 hours.

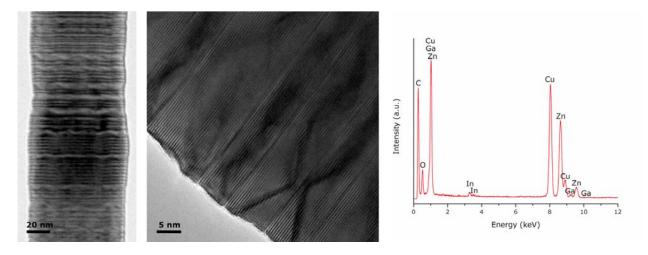


Figure S2: Indium gallium zinc oxide (IGZO) nanowires. TEM images and EDS spectrum of IGZO nanowires prepared by coating ZnO nanowires with 10 nm of In and 10 nm of Ga and annealing at 1173 K in oxygen for 12 hours. The In:Ga ratios were approximately 1:1 by EDS in all the nanowires. For example, in the 10/10 IGZO nanowires, the atomic percentages of In, Ga, and Zn in a 110 nm nanowire were 6.3, 6.0, and 87.7, respectively.

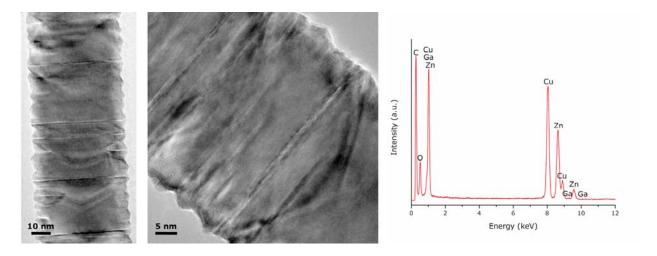


Figure S3: Gallium zinc oxide (GZO) nanowires. TEM images and EDS spectrum of GZO nanowires prepared by coating ZnO nanowires with 10 nm of Ga and annealing at 1173 K in oxygen for 12 hours.

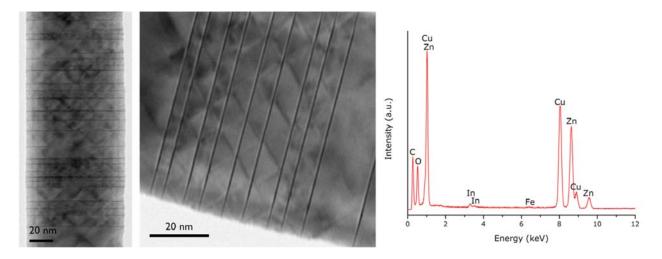


Figure S4: Indium iron zinc oxide (IFZO) nanowires. TEM images and EDS spectrum of IFZO nanowires prepared by coating ZnO nanowires with 5 nm of In and 5 nm of Fe and annealing at 1173 K in oxygen for 12 hours.

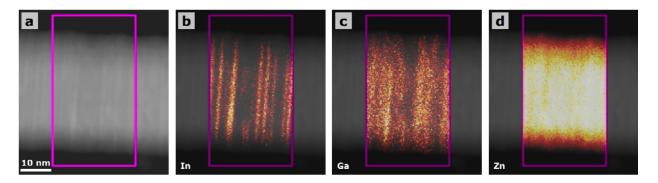


Figure S5: Elemental mapping. a, STEM image of an IGZO nanowire and the corresponding EDS element maps for In (**b**), Ga (**c**), and Zn (**d**) overlaid on the original image.

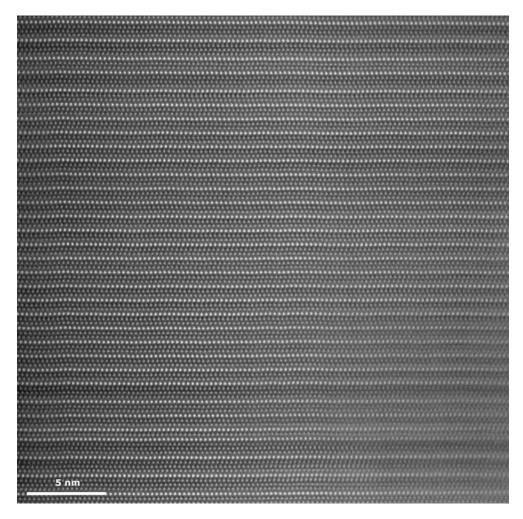


Figure S6: 40/40 indium gallium zinc oxide nanowires. Z-contrast STEM image showing a high density of inclusions layers with spacings corresponding to n=2 and n=1.

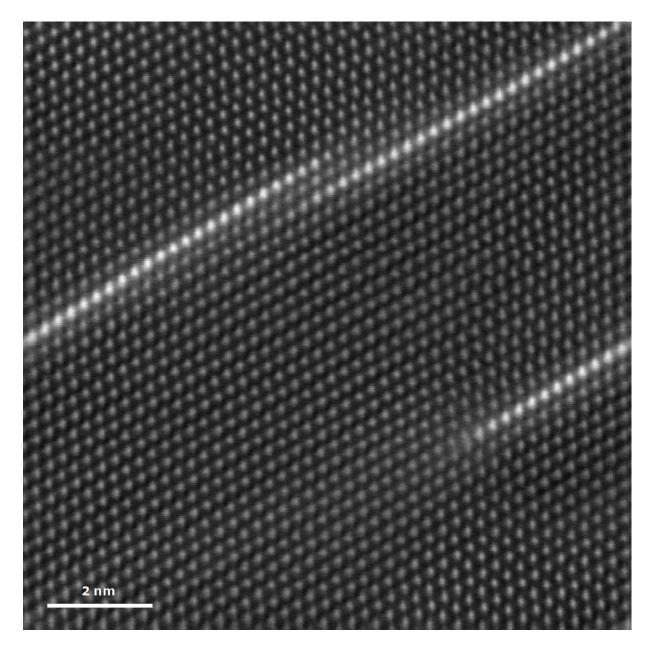


Figure S7: Partial inclusions merge together. Z-contrast HRSTEM image of IGZO showing three partial inclusions. The two partial inclusions at the top of the image appear to be merging together via edge dislocation climb to create a single complete inclusion layer.

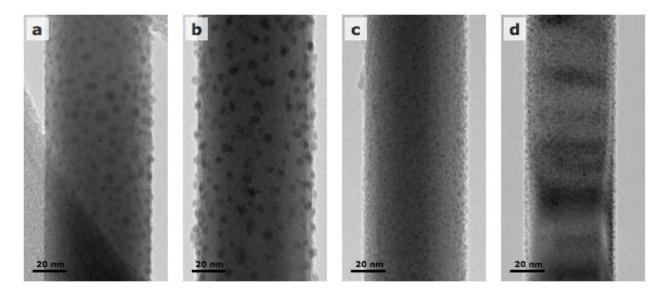


Figure S8: Pre-annealed TEMs. ZnO nanowires coated with 5 nm of In and 5 nm of Ga (a), 10 nm of In (b), 10 nm of Ga (c), and 5 nm of In and 5 nm of Fe (d)