

Synergistic Combination of Atomic Scale Structural Engineering and Panoscopic Approach in p-type ZrCoSb-based half-Heusler thermoelectric materials for high ZT”.

N. S. Chauhan^{1,2}, A. Bhardwaj^{1,2}, T. D. Senguttuvan^{1,2}, R. P. Pant^{2,3}, R.C. Mallik⁴ and D. K. Misra*^{1,2}

¹Physics of Energy Harvesting Division, CSIR-National Physical Laboratory, Dr. K.S. Krishnan Marg, New Delhi-110012.

²Academy of Scientific & Innovative Research (AcSIR), CSIR-National Physical Laboratory (CSIR-NPL) Campus, New Delhi-110012, India.

³EPR Spectroscopy Section, CSIR-National Physical Laboratory, Dr. K.S. Krishnan Marg, New Delhi-110012.

⁴Department of Physics, Indian Institute of Science, Bangalore, 560 012, India.

SUPPLEMENTARY INFORMATION

The SEM morphologies and corresponding energy dispersive X-ray analysis (EDAX) spectrum recorded from the each of the composition of $\text{ZrCo}_{1+x}\text{Sb}_{0.9}\text{Sn}_{0.1}$ ($x=0.01, 0.03, 0.05$ and 0.07) are shown in Fig S1 indicating a clear two phase contrast and compositions very close to their respective nominal compositions. Figure S1(a, b, c & d) envisages the increasing FH inclusions within the HH matrix with increasing content of excess Co in compositions $\text{ZrCo}_{1+x}\text{Sb}_{0.9}\text{Sn}_{0.1}$ ($x=0.01, 0.03, 0.05$ and 0.07). Interestingly, one can clearly notice the increasing size of FH inclusions and its multiple length scales (S1c, e & f) with increasing FH fractions. The compositional analysis was performed employing EDAX to verify the homogeneities of the samples. A representative EDS spectrum and quantification of elements of $\text{ZrCo}_{1+x}\text{Sb}_{0.9}\text{Sn}_{0.1}$ ($x=0.01, 0.03, 0.05$ and 0.07) have been displayed in Fig S1 showing all constituent elements and quantification of composition obtained from the average of values taken at 8 positions shown in the Insets reveals compositions close to the corresponding nominal compositions. The compositions of HH and FH in all the compositions $\text{ZrCo}_{1+x}\text{Sb}_{0.9}\text{Sn}_{0.1}$ have been quantified and averaged from values taken at 8 positions and no obvious impurities phase were observed other than HH and FH in any of the composite samples. A representative EDS spectrum and quantification of elements for the best performing sample $\text{ZrCo}_{1+x}\text{Sb}_{0.9}\text{Sn}_{0.1}$ have been presented for each composition.

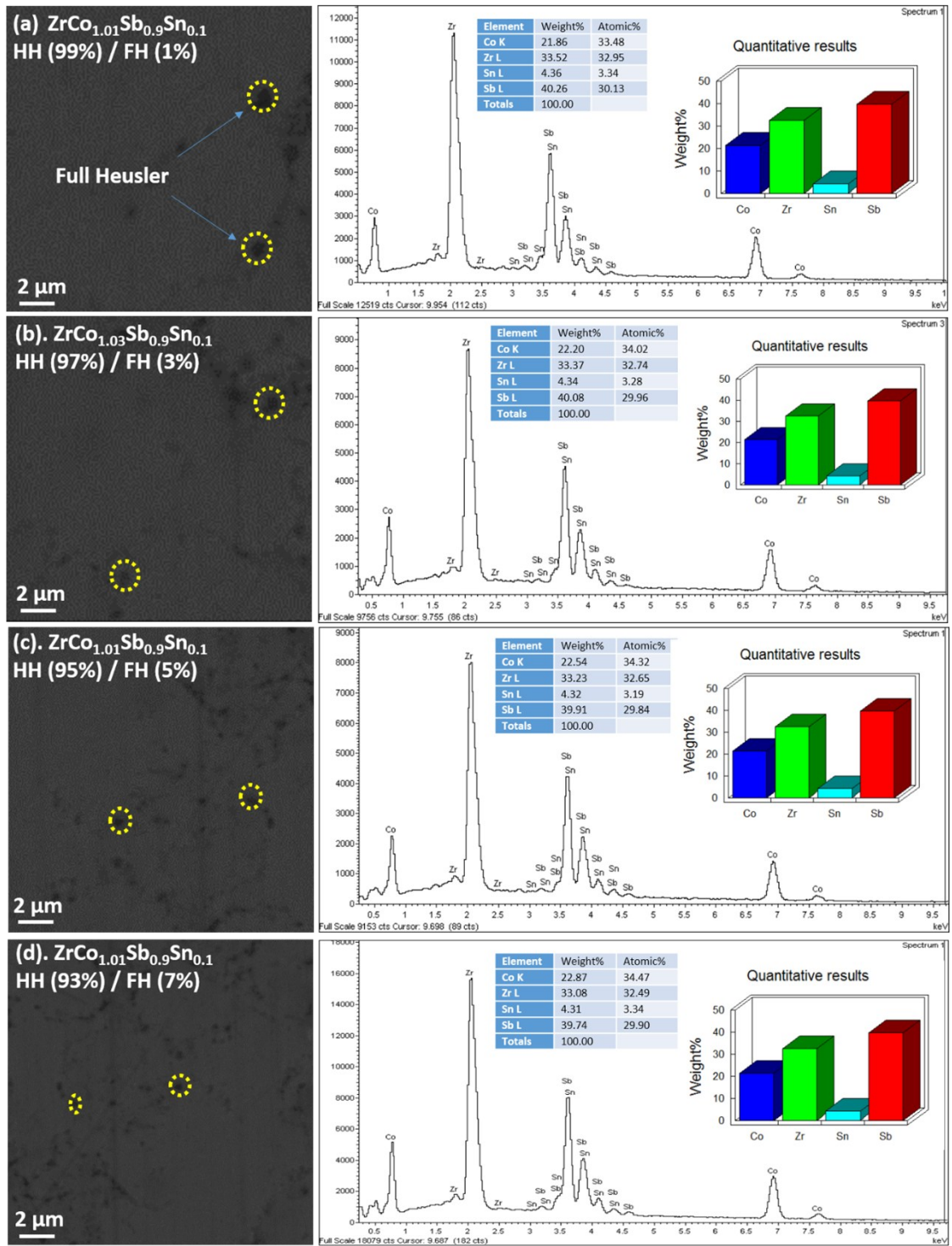


Figure. S1. The back scattered SEM micrograph along with representative EDS spectrum and quantification of elements of HH (1-x)/FH(x), $ZrCo_{1+x}Sb_{0.9}Sn_{0.1}$ ($x=0.01, 0.03, 0.05$ and 0.07)