Supporting Information -

Non-stoichiometry in the Zintl phase Yb$_{1-\delta}$Zn$_2$Sb$_2$ as a route to thermoelectric optimization

Alex Zevalkink,[†,‡] Wolfgang G. Zeier,[†] Ethan Cheng,[‡] Jeffrey Snyder,[∗,†]

Jean-Pierre Fleurial,[‡] and Sabah Bux[∗,‡]

Material Science, California Institute of Technology, Pasadena, CA, USA, and Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, USA

E-mail: jsnyder@caltech.edu; sabah.k.bux@jpl.nasa.gov

[∗]To whom correspondence should be addressed
[†]Material Science, California Institute of Technology
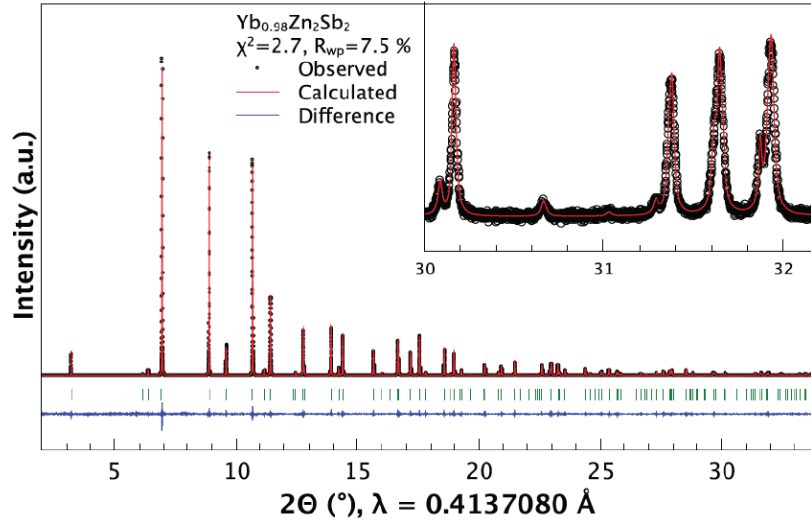[‡]Thermal Energy Conversion Technologies Group

Figure S 1: Synchrotron diffraction data of nominal $Yb_{0.98}Zn_2Sb_2$, including profile fit, profile difference and profile residuals (χ^2 and R_{wp}) of the corresponding Rietveld refinement. The inset shows the goodness-of-fit at high angles.
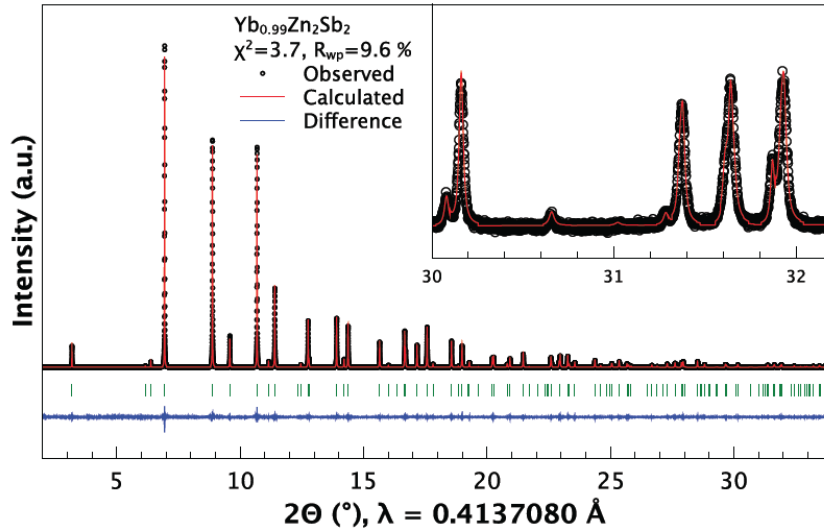

Figure S 2: Synchrotron diffraction data of nominal $Yb_{0.99}Zn_2Sb_2$, including profile fit, profile difference and profile residuals (χ^2 and R_{wp}) of the corresponding Rietveld refinement. The inset shows the goodness-of-fit at high angles.
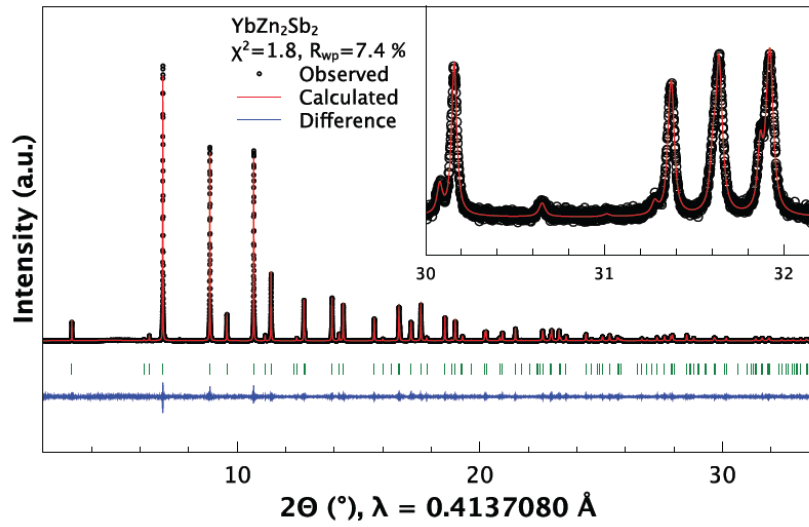
Figure S 3: Synchrotron diffraction data of nominal $Yb_{1.00}Zn_2Sb_2$, including profile fit, profile difference and profile residuals (χ^2 and R_{wp}) of the corresponding Rietveld refinement. The inset shows the goodness-of-fit at high angles.
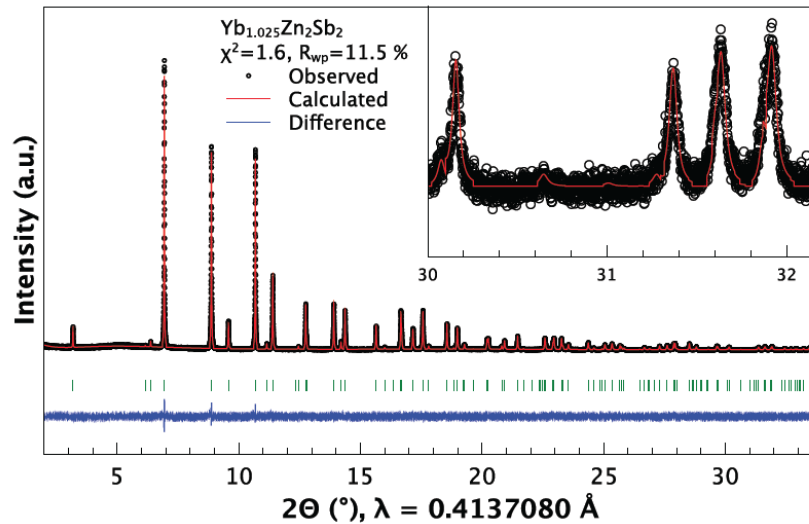

Figure S 4: Synchrotron diffraction data of nominal $Yb_{1.025}Zn_2Sb_2$, including profile fit, profile difference and profile residuals (χ^2 and R_{wp}) of the corresponding Rietveld refinement. The inset shows the goodness-of-fit at high angles.
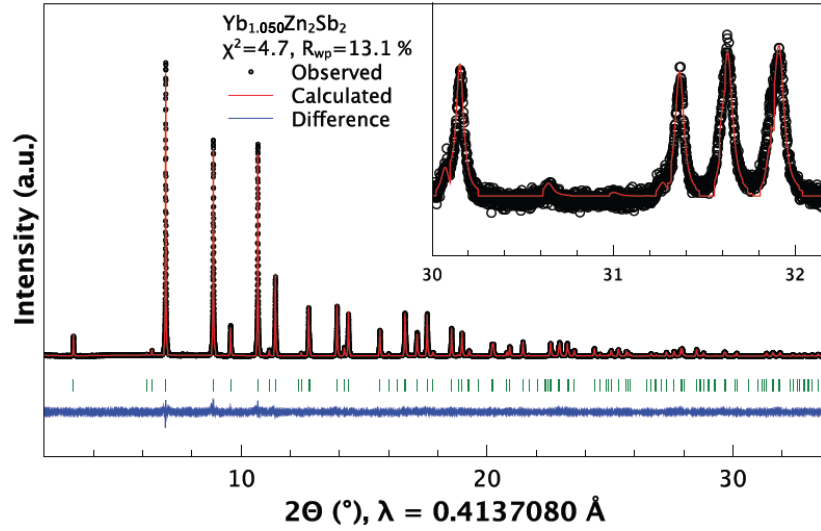
Figure S 5: Representative synchrotron diffraction data of $Yb_{1.05}Zn_2Sb_2$, including profile fit, profile difference and profile residuals (χ^2 and R_{wp}) of the corresponding Rietveld refinement. The inset shows the goodness-of-fit at high angles.
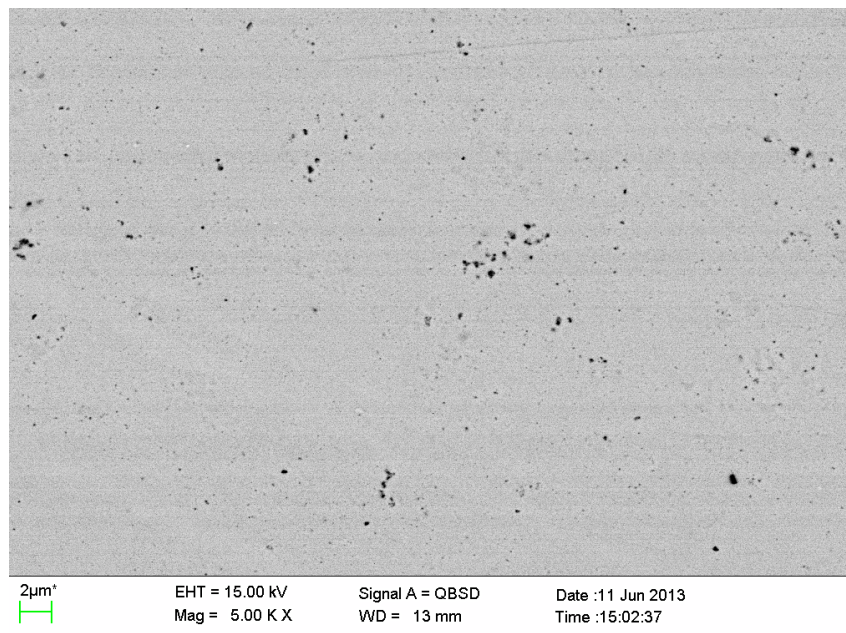

Figure S 6: Back-scattered SEM image of sample with $x = 0.98$. The black spots were identified as pores.
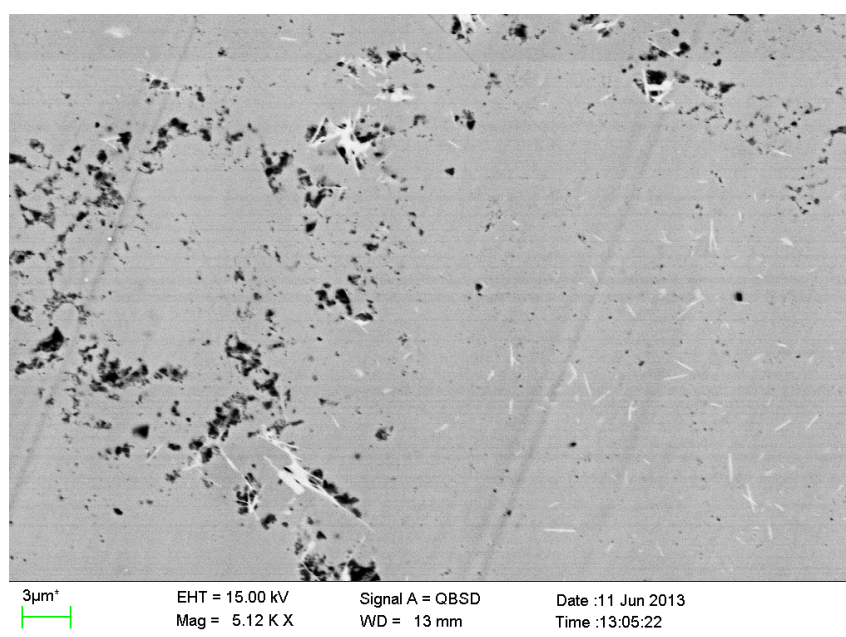
Figure S 7: Back-scattered SEM image of sample with $x = 1.05$. The black spots were identified as pores and white needles are a Yb-rich secondary phase.