Supplementary Material for

Disordered Zinc in Zn_4Sb_3 with Phonon Glass, Electron Crystal Thermoelectric Properties

G. Jeffrey Snyder,[1,2] Mogens Christensen,[3] Eiji Nishibori,[4] Thierry Caillat,[2] Bo Brummerstedt Iversen[3]

[1]*California Institute of Technology, Materials Science, 1200 East California Boulevard, Pasadena, CA 91125, USA*

[2]*Jet Propulsion Laboratory/California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109, USA*

[3] *Department of Chemistry, University of Aarhus, DK-8000 Aarhus, Denmark*

[4] *Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan*

Single Crystal Structure Refinement

The single crystal data collection parameters and results of the final model are summarized in Table S1. The shortest interatomic distances are tabulated in Table S2. The thermal displacement ellipsoids are shown in Figure S1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2a^{*2}U_{11} + ... + 2\, h\, k\, a^*\, b^*\, U_{12}\,]$.

The synchrotron X-ray powder diffraction data of Zn_4Sb_3 compared to the Rietveld solution is given in Figure S2.

Table S1. Single crystal data collection and structure refinement for Zn_4Sb_3.

Temperature	293(2) K
Wavelength	0.71073 Å
Theta range for data collection	3.33° to 38.21°
Index Ranges (96.3 % complete to 38.21°)	$-21 \le h \le 21$ $-20 \le k \le 20$ $-18 \le l \le 18$
R_σ (14773 reflections collected)	1.64%
R_{int} (956 independent reflections)	4.24%
Refinement method	Full-matrix least-squares on F^2
Weighting Scheme	$1/(\sigma^2 + 25\ P)$ $P = (Max(I_o,0)+2\ I_c) / 3$
R indices ($I > 2\ \sigma(I)$)	R1 = 2.57%, wR2 = 4.56%
R indices (all data)	R1 = 3.03%, wR2 = 4.59%
Data / restraints / parameters	956 / 19 / 50
Largest difference peak and hole	1.941 and -1.577 e / $Å^3$
Absorption coefficient	26.586 mm^{-1}
Extinction coefficient	0.00044(2)

Table S2. Interatomic distances (Å) for Zn_4Sb_3. Zinc interstitial distances to other zinc atoms are omitted.

Sb(1) – Zn(1) × 2	2.7262(7)
Sb(1) – Zn(1) × 2	2.7816(7)
Sb(1) – Zn(1) × 2	2.7940(7)
Sb(2) – Zn(1) × 3	2.6814(7)
Sb(2) – Sb(2)	2.8183(7)
Zn(1) – Sb(2)	2.6814(7)
Zn(1) – Sb(1)	2.7262(7)
Zn(1) – Sb(1)	2.7816(7)
Zn(1) – Sb(1)	2.7940(7)
Zn(1) – Zn(1)	2.7738(15)
Zn(2) – Sb(1)	2.59(2)
Zn(2) – Sb(1)	2.71(2)
Zn(2) – Sb(1)	2.78(2)
Zn(2) – Sb(2)	2.73(2)
Zn(3) – Sb(1)	2.65(2)
Zn(3) – Sb(1)	2.56(1)
Zn(3) – Sb(2)	2.54(2)
Zn(3) – Sb(2)	3.03(5)
Zn(4) – Sb(1)	2.61(2)
Zn(4) – Sb(1)	2.83(3)
Zn(4) – Sb(2)	2.73(2)
Zn(4) – Sb(2)	3.05(3)
Zn(4) – Sb(1)	3.10(4)

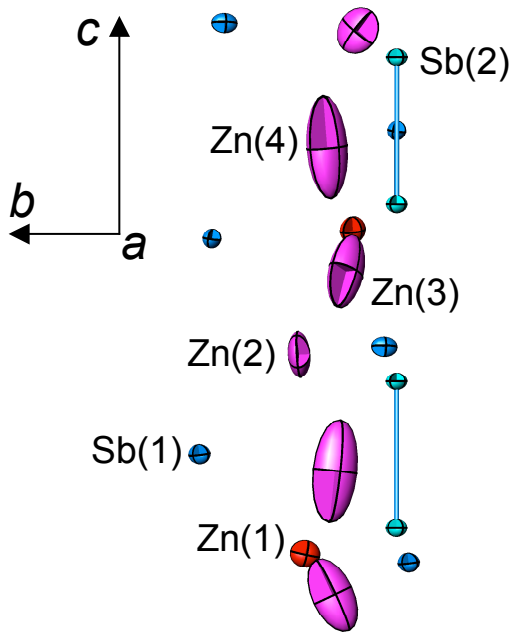

Figure S1. View along *a* (*c* is vertical) of anisotropic thermal displacement ellipsoids for the model of Zn_4Sb_3 with interstitials. The interstitial ellipsoids are large and elongated along *c* in the direction of a nearby Zn(1) or Zn-interstitial.

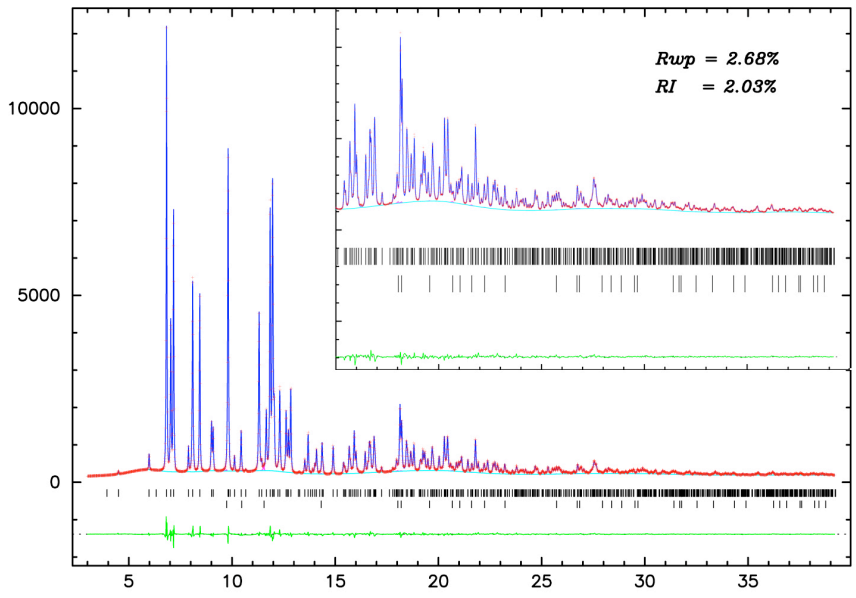

Figure S2. Synchrotron X-ray powder diffraction of Zn_4Sb_3. The lower green curve is the difference between the observed intensity and the interstitial model after Rietveld analysis.