Supporting Information

Composition Modulation of Ag_2Te Nanowires for Tunable Electrical and Thermal Properties

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This document includes the details of the experiments and the procedures for the theoretical modeling of the thermoelectric properties. Besides, the supplementary Figure S1 shows the XRD pattern of the Ag_2Te nanowires synthesized with stoichiometric amount of Ag precursor.

Experiments and Modeling Procedures

Synthesis of Ag_2Te nanowires. All chemicals are used as received without further purification. TeO_2 (≥99%), Polyvinylpyrrolidone (PVP for short, MW~40,000), KOH (90%), N_2H_4•H_2O (78%~82%), are purchased from Sigma Aldrich, while $AgNO_3$ (≥99.9%), ethylene glycol (≥99%, EG for short) and ethanol (95%) are purchased from VWR. In the first step of a typical synthesis, 9.576 g TeO2, 12 g PVP, 44.884 g KOH, and 600 ml ethylene glycol are added to a one-liter glass reactor. The mixture is heated to 120 °C with vigorous stirring and all solids are dissolved. Then, the reactor is purged with nitrogen using a Schlenk line, and 20 ml N_2H_4•H_2O is injected rapidly. The mixture is kept at 120 °C for 1 hour for Te nanowire growth, and is let cool down to room temperature naturally. The products are triple washed with distilled water, collected with centrifugation and re-dispersed in 800 ml ethylene glycol in a 2 L beaker for the second step. In a separate 500 mL beaker, 40.769 g (for Ag_2Te_2xAg sample) or 61.153 g (for Ag_2Te_3xAg sample) $AgNO_3$ is dissolved in 200 ml ethylene glycol. Then, the $AgNO_3$/EG solution is added into the 2 L beaker, and the mixture is stirred vigorously at room temperature for two hours for the conversion from Te into Ag_2Te. The products are triple washed with DI water and collected with centrifugation for future use. The yield of Ag_2Te nanowires is estimated to be ~44% calculated from the initial amount of the tellurium precursor (TeO_2).

Hydrazine treatment and hot press. To remove the surface ligands, the Ag_2Te nanowires are dispersed in 800 ml ethanol and mixed with 80 ml N_2H_4•H_2O under vigorous stirring for a day. [1-3] The nanowires are then collected with centrifugation and washed with DI water for three times. They are then dried at room temperature under vacuum and ground into loose powder in a nitrogen-filled glove box. For hot press, around 4 g nanowire powder is loaded into a 0.73 inch diameter stainless die in the glove box, compressed at a pressure of 165 MPa, heated to 150 °C and held at the same temperature for 20 minutes, and then cooled down to room temperature naturally.

Measurements of thermoelectric properties. The Seebeck coefficients of the hot-pressed samples are measured with a home-built Seebeck measurement system operated under vacuum, in which two heaters are used to control the overall temperature and to generate temperature difference between the hot and cold sides of the sample, and two type-K thermocouples are used to measure temperature and the voltage differences between the hot and cold sides of the sample. The electrical conductivity and Hall coefficients are measured on a custom-built Hall apparatus using van der Pauw geometry, and a 2 T magnetic field is used for Hall coefficient measurements.[4] Thermal diffusivity (a) measurements are completed using the laser flash method. Density (ρ) is determined by measuring sample dimensions and mass. Then thermal conductivity is calculated from the equation $\kappa = a * C_p * \rho$, where C_p stands for specific heat and the Dulong-Petit value ($3k_BT$ per atom) is used for C_p. The same treatment for C_p has been reported in several papers on Ag_2Te.[5-7]

Modeling with Boltzmann Transport Equations. We also model the charge carrier transport for the materials in ambipolar transport regime using the near-equilibrium Boltzmann transport equations under the relaxation time approximation. More information about the modeling is found in previous report.[8] The band structure of Ag_2Te is modeled based on the Kane model with nonparabolic energy dispersion since the bands of Ag_2Te were found to be nonparabolic.[5] The scattering characteristic is found by fitting the experimental mobility of each sample. The acoustic phonon scattering is taken into account as the predominant scattering mechanism in Ag_2Te. The additional scattering by nanostructuring and compositional variation in the material is accounted for using the ionized impurity scattering and the short-range defect scattering with the adjustable parameters therein.

Supplementary Figure

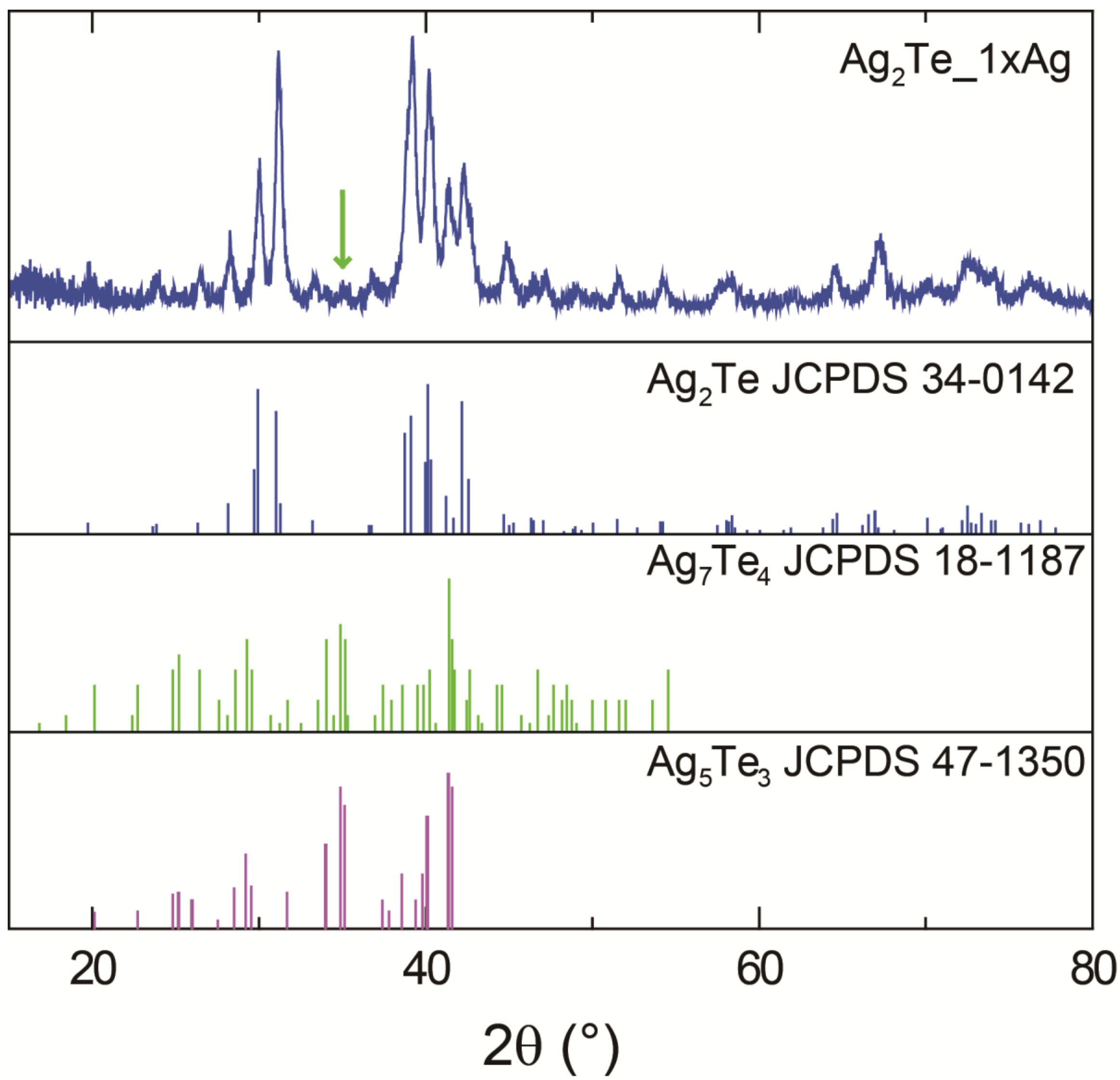

Figure S1. XRD pattern of the Ag_2Te nanowires synthesized with stoichiometric amount of Ag precursor compared to the standard power XRD patterns of Ag_2Te, Ag_7Te_4, and Ag_5Te_3. The peaks indicated by the arrow are attributed to the existence of Ag_7Te_4 or Ag_5Te_3.

Supplementary Reference

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