Synergistic enhancement of thermoelectric and mechanical properties in Bi-Sb-Te alloys collaborated by Zn based metal organic Framework (ZIF-8)

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Experiment Details

The phase structures of all samples were characterized by X-ray diffraction (XRD, MiniFlex 600 Rigaku, Japan) with Cu Ka radiation (1.5406Å). The microstructure of the samples was detected via field emission scanning electron microscopy (FESEM, ZEISS, Sigma 300, German), and the element distribution in the samples was studied by energy dispersive spectroscopy (EDS, JED-2300 T). Fine nano-scale microstructural characterization was characterized using high-resolution transmission electron microscopy (HRTEM, JEOL JEM-F200, Japan). The electrical performance measurements adopt the ZEM3 Seebeck and resistance test system produced by Company Ulvac-Riko, Japan. The total thermal conductivity (κ_{tot}) can be obtained by the formula $\kappa_{tot} = \rho D C_p$, where the density (ρ) is obtained from Archimedes method, the thermal diffusion coefficient(D) was obtained using LFA467 measurement system (NETZSCH, Germany), the heat capacity $({}^{C}_{p})$ is calculated by Feng' First-principle calculation¹. The carrier concentration (n) and mobility (μ) were obtained by the roomtemperature Hall effect measurement system (Ecopia, HMS-700, Republic of Korea) at a magnetic field of 0.5T and a current of 30mA. The sound velocity of all samples was measured using ultrasonic scattering method (UMS-100, TECLAB, France). The power generation performance of the single-leg device was tested using the Mini-PEM from Advance Riko. We selected the 0.3 wt.% ZIF-8 doped sample as the single-leg device particle, and then prepared the contacting layer (Ni) on the upper and lower surfaces of the sample by electroplating. In order to further reduce the contact resistance at the interface, silver pastes were added between the Cu sheet and the Ni layer as a connecting layer. Before welding, we used 2000-mesh sandpaper to slightly polish the copper electrode to increase the bonding force between the electrode and the

thermoelectric particles. The prepared single-leg thermoelectric device was set up on the Mini-PEM instrument (Illustration of Fig. 8c), and silicone grease was applied to the Cu sheet at the high-temperature end to improve thermal conductivity. The cold-side temperature (^{T}c) was maintained at 298K, and the hot-side temperatures (^{T}h) are set to 348K, 398K, 448K, 498K and 548K, respectively. The measurement results were provided in terms of output voltage, output power, and conversion efficiency. The mechanical properties of the samples including Vickers hardness and Young's modulus were obtained by nanoindentation method (iMicro KLA, USA). Two samples of pure sample and optimal thermoelectric performance (0.3 wt%) were selected as measurements objects. After the samples were precisely polished, the square area of 300 µm×300 µm (with 900 points) is selected on the surface to obtain mechanical properties under the condition that the radius of curvature of the tip is 20nm and the load is 20mN.



Fig.S1 Powder XRD patterns of ZIF-8. This result indicates that the doped ZIF-8 is pure phase, and there is no impurity phase^{2–5}.



Fig.S2 The structure diagram of ZIF-8, which indicates that ZIF-8 has a shell structure.



Fig.S3 SEM image of ZIF-8.



Fig.S4 Image of a nanopore in the 0.3 wt% ZIF-8 sample in TEM mode with EDS elemental mapping. This result illustrates that the $Zn_{Bi,Sb}$ defect clusters are not localized, but are widely distributed near the holes.⁶

References

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