Supporting Information

Hammering Ag_2Se thermoelectric materials into complex conformal shape with maintained Harman zT

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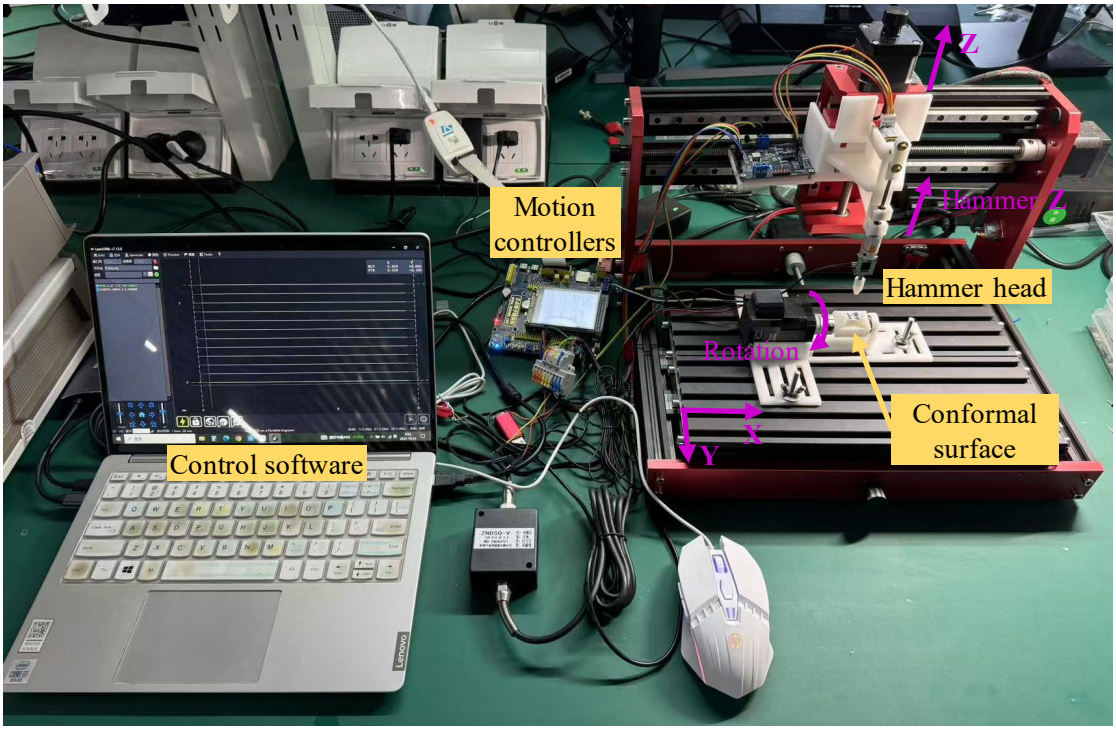

Fig. S1. Home-made hammering equipment.

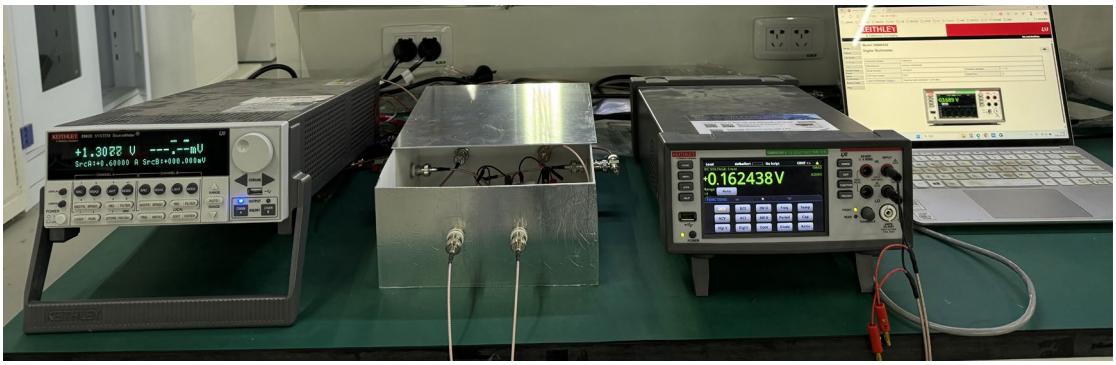

Fig. S2. Home-made Harman *zT* platform.

$$S_t = S_g + \left(S_{gb} - S_g\right)\frac{\Delta T_{gb}}{\Delta T_t} \qquad \text{(S1)}$$

Here, S_t is total Seebeck coefficient of the Ag_2Se sample, S_g is Seebeck coefficient of the Ag_2Se single crystal. S_{gb} is Seebeck coefficient of the Ag_2Se grain boundary phase.

$$S_{gb} = S_g + \left(S_t - S_g\right)\frac{k_g}{k_g - k_t} \qquad \text{(S2)}$$

Here, S_g and k_g are Seebeck coefficient and thermal conductivity of Ag_2Se single crystal, which are measured and its values are based on references. Corresponding S_t and k_t are those of Ag_2Se polycrystalline.

$$\frac{\Delta T_{gb}}{\Delta T_t} = \frac{1}{\frac{d}{k_g \rho_{Kapitza}} + 1} \qquad \text{(S3)}$$

$$\rho_{Kapitza} = d\left(\frac{1}{k_t} - \frac{1}{k_g}\right) \qquad \text{(S4)}$$

Here, d is average grain size.

$$\sigma_t = \frac{\sigma_g}{1 + \frac{\rho_{el-gb}\sigma_g}{d}} \qquad \text{(S5)}$$

Here, ρ_{el-gb} is electrical interface resistivity of Ag_2Se grain boundary phase. ρ_{el-gb} is calculated by the following formula,

$$\frac{1}{\rho_{Kapitza}} = L\frac{1}{\rho_{el-gb}}T + \frac{1}{\rho_{Lattice-gb}} \qquad \text{(S6)}$$

Here, $\rho_{Lattice-gb}$ is the thermal resistivity contribution from lattice at the grain boundary, $\rho_{Lattice-gb}$ parameter is used as a fitting parameter in our calculation.

$$k_t = \frac{k_g}{1 + \frac{\rho_{Kapitza} k_g}{d}} \qquad \text{(S7)}$$

The power factor *PF* and thermoelectric figure of merit (*zT*) of the hammered Ag_2Se samples with different grain sizes are calculated based on the above calculated Seebeck coefficient, electrical conductivity, and thermal conductivity.

$$PF = S_t^2 \sigma_t \quad \text{(S8)}$$

$$zT = \frac{S_t^2 \sigma_t}{k_t} T \quad \text{(S9)}$$

Here, *T* is the absolute temperature, in our study, only room temperature is considered.

Table S1. Calculated parameters for Ag_2Se single crystal parallel to (201) plane.

Parameters	Value	Reference
$\boldsymbol{S_g}$	-147 μV/K	[1]
$\boldsymbol{k_g}$	1.31 W/mK	[1]
$\boldsymbol{\sigma_g}$	$1.01*10^5$ S/m	[1]

Table S2. Calculated parameters for $Ag_{21}Se$ single crystal perpendicular to (201) plane.

Parameters	Value	Reference
$\boldsymbol{S_g}$	-122 μV/K	[1]
$\boldsymbol{k_g}$	1.03 W/mK	[1]
$\boldsymbol{\sigma_g}$	$1.51*10^5$ S/m	[1]

Table S3. Calculated parameters for Ag_2Se polycrystalline.

Parameters	Value	Reference
$\boldsymbol{S_t}$	-170 μV/K	[2]
$\boldsymbol{k_t}$	0.92 W/mK	[2]

Table S4. Fitting parameter $\rho_{Lattice-gb}$ values.

Ag_2Se parallel to (201) plane	Ag_2Se vertical to (201) plane	average of single crystal Ag_2Se parallel and vertical to (201) plane
$1.5*10^{-6.5}$	$1.4*10^{-7}$	$1.5*10^{-8}$
$1.5*10^{-6}$	$1.4*10^{-8}$	$1.5*10^{-6}$
$1.5*10^{-4}$	$1.4*10^{-6}$	$1.5*10^{-7}$

Molecular dynamics (MD) simulation

The computational domain for MD simulations had x/y/z dimensions of 10 nm, 10 nm, and 100 nm, respectively. Both the hot and cold ends are geometrically 1 nm*1 nm*1 nm.

Reference

[1] Lin S, Guo L, Wang X, et al. Revealing the promising near-room-temperature thermoelectric performance in Ag_2Se single crystals[J]. Journal of Materiomics, 2023, 9(4): 754-761.

[2] Kleinhanns T, Milillo F, Calcabrini M, et al. A Route to High Thermoelectric Performance: Solution‐Based Control of Microstructure and Composition in Ag_2Se[J]. Advanced Energy Materials, 2024, 14(22): 2400408.