Enhancement of Anisotropic Thermoelectric Performance of Tungsten Disulfide by Titanium Doping

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Electronic Supplementary Information

Fig. S1 (a) TEM image of Ti_{0.1}WS_2, (b) electron diffraction pattern of area marked by red rectangle in (a), (c) HRTEM image of area marked by red rectangle in (a).

Fig. S2 (a) SEM image of polished Ti_{0.1}WS_2, (b-d) EDX elemental mapping of Ti_{0.1}WS_2, (b) Sulfur elemental mapping, (c) Titanium mapping, (d) Tungsten mapping.

Fig. S3 Electronic band structure and DOS for (a) pristine WS_2 and (b) Ti doped WS_2 supercell.

Fig. S4 (a) XRD pattern for Ti_xWS_2 (x=0, 0.02, 0.05, 0.1, 0.15, 0.20) along the direction perpendicular to pressing direction, (b) an enlarged view of XRD pattern around TiW alloy peak.

Calculation of Ti distribution

The distribution of Ti atoms in Ti_xWS_2 was calculated using XRD data. First, the mass ratio of TiW alloy (as second phase) was
calculated using relative intensity ratio (RIR) method.\textsuperscript{19} The following equation was used:

\[ W_B = \frac{I_B}{I_B + I_A K_B^A} \]  \hspace{1cm} (3)

where \( W_B \) is the mass ratio of TiW phase, \( I_B \) is the integrated intensity of the strongest peak of TiW phase, \( I_A \) is the integrated intensity of the strongest peak of WS\(_2\) phase, \( K_B^A \) is the RIR ratio of two phases. Then the molar ratio of TiW/WS\(_2\) (a) was calculated using

\[ a = W_B x (M_1 + M_2)/M_3 \]

where \( x \) is the total molar ratio of Ti atoms in samples, \( M_1 \) is the molar mass of Ti atom, \( M_2 \) is the molar mass of WS\(_2\), \( M_3 \) is the molar mass of TiW. The molar ratio of Ti atoms (b) in lattice was calculated using

\[ b = x - a \]

\( x \) values are 0.02, 0.05, 0.1, 0.15, 0.2.

<table>
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<th>0.02</th>
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</tbody>
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Table S1, Molar ratio of TiW phase (a) and Ti atoms in lattice (b).