Supplementary information

Thermal Rectifier and Thermal Transistor of 1T/2H MoS_2 for Heat Flow Management

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1.Lithium insertion method

Firstly, 2H-MoS_2 film is placed into 10 ml 2.5M n-butyl lithium solution for 10 hours. During the immersion process, the 2H-MoS_2 will gradually be transformed into 1T phase. Then n-butyl lithium is removed by using n-ethane. Finally, 1T-MoS_2 is rinsed with deionized water and dried. The process is conducted in a glove box under an argon atmosphere to prevent the reaction between lithium ions and air.

2. Work function measurement

The work function of the obtained 2H- and 1T- MoS_2 films were measured to illustrate the phase transition between the two phases. The model of ultraviolet photoelectron spectrometer (UPS) detection is AXIS ULTRA DLD of Kratos company. The ultraviolet source is nonmonochromatic He I and the energy of the He I source is 21.2 eV. According to the UPS results of 2H- and 1T-MoS_2 films, it can be seen that the work function of 2H-MoS_2 is ~ 4.3 eV. While the work function of 1T-MoS_2 is ~3.0 eV. It also shows that phase transition has taken place between the two phases.

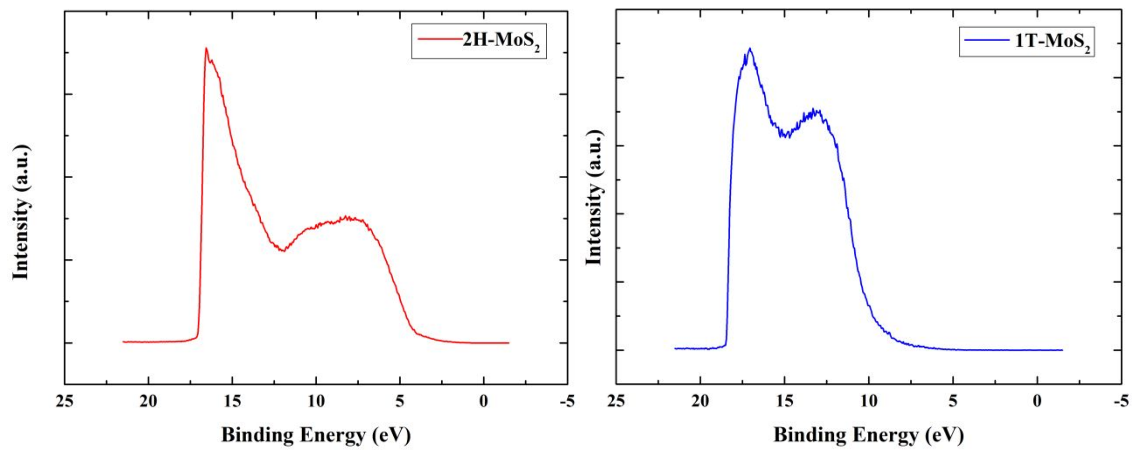

Figure S1. UPS results of 2H- and 1T- MoS_2 films

3. Calculation

The thermal conductivity of the MoS_2 film is calculated by equation 1 [1]. Equation 4 is used to calculate the experimental thermal rectification coefficient [2].

$$\lambda = \frac{QL_s}{\Delta TA} = \frac{U_1^2}{R_1} \cdot \frac{T_2}{(T_1 + T_2)} \cdot \frac{L_s}{A\Delta T} = \frac{U_1^2 T_2 L_s}{R_1(T_1 + T_2)A(T_1 - T_2)} \tag{1}$$

$$T_1 = \frac{(R_1/R_0 - 1)}{\alpha} \tag{2}$$

$$T_2 = \frac{(R_2/R_0 - 1)}{\alpha} \tag{3}$$

where λ, L_s and A are the thermal conductivity, length and cross-sectional area of the sample, respectively. Q is the heat transfer rate. U_1 is the voltage of the heating electrode. ΔT is the temperature difference across the sample. T_1 and T_2 are the temperature of the heating electrode and the heat receiving electrode. R_0 is the initial resistance, and R_1 and R_2 are the resistance of the two electrodes after heating. α is the temperature coefficient of resistance of the electrode.

$$\eta = \frac{|\lambda_p - \lambda_n|}{\lambda_p} \cdot 100\% \tag{4}$$

where η, λ_p , and λ_n are the thermal rectification coefficient, the thermal conductivity in positive direction, and the thermal conductivity in negative direction, respectively.

4. Calculation of contact thermal resistance

In this work, the MoS_2 films were transferred to microelectrodes by PMMA and directly contact with metal film. Hence, it is necessary to analyze the effect of contact thermal resistance on thermal conductivity. Here, a fin thermal resistance model was applied [3].

$$R_c = [\lambda A m \tanh(mL_c)]^{-1} \tag{5}$$

$$m = \sqrt{\frac{w}{\lambda A R_i}} \tag{6}$$

where A, λ and w are the cross-sectional area, thermal conductivity and width of the MoS_2 film ($A = wt$, t is the thickness of MoS_2 film), R_c is the contact thermal resistance, R_i is the interfacial thermal resistance per unit area ($R_i = 7.14\times10^{-8}$ m^2K/W) [4], L_c is the contact length between MoS_2 film and microelectrode. The calculated results are summarized in Tables S1.

Table S1 Contact thermal resistances of MoS_2 film

MoS_2 film	Lc (μm)	L (μm)	w (μm)	λ ($Wm^{-1}K^{-1}$)	d (nm)	$R_0 \times 10^5$ (KW^{-1})	$R_c \times 10^5$ (KW^{-1})	R_c / R_0 (100%)
1	1	1.65	2.67	50	6.5	19.01	1.75	9.23
2	1	1.66	8.47	35	6.5	8.61	0.66	7.66

Table S1 shows the contact thermal resistances of experimental MoS_2 samples. There was ~ 8.4% of the average thermal resistance of MoS_2 samples. It can explain that the contact thermal resistant has a little effect on the thermal conductivity. There is however no influence on the thermal rectification because the nearly same heat flow are cross the sample in the opposite directions [1].

5. Model simulation

The thermal analysis results of five thermal rectifier were conducted by COMSOL Multiphysics^{TM} as shown in **Figure S2**(a-e). The first had the positive 2H phase of sample 1 on the left and the negative 2H phase of sample 1 on the right; the second had the positive 1T phase of sample 1 on the left and the negative 2H phase of sample 1 on the right; the third had the positive 2H phase of sample 2 on the right and the negative 2H phase of sample 2 on the right; the fourth was the positive 1T phase of sample 2 on the left and the negative 2H phase of sample 2 on the right; the fifth was the positive 1T phase of sample 2 on the left and the negative 2H phase of sample 1 on the right. The geometric sizes of MoS_2 films and microelectrodes were measured based on their SEM images. In the thermal analysis model, the temperature of the middle electrode was set to 333.15 K, and the initial temperature of the left and right electrodes was 293.15 K. Other surfaces were thermal insulation. The thermal conductivity of MoS_2 samples were also determined according to the experimental value. The heat flow transferred among the cross-plane direction and the temperature difference of left and right electrodes were the unknown parameter.

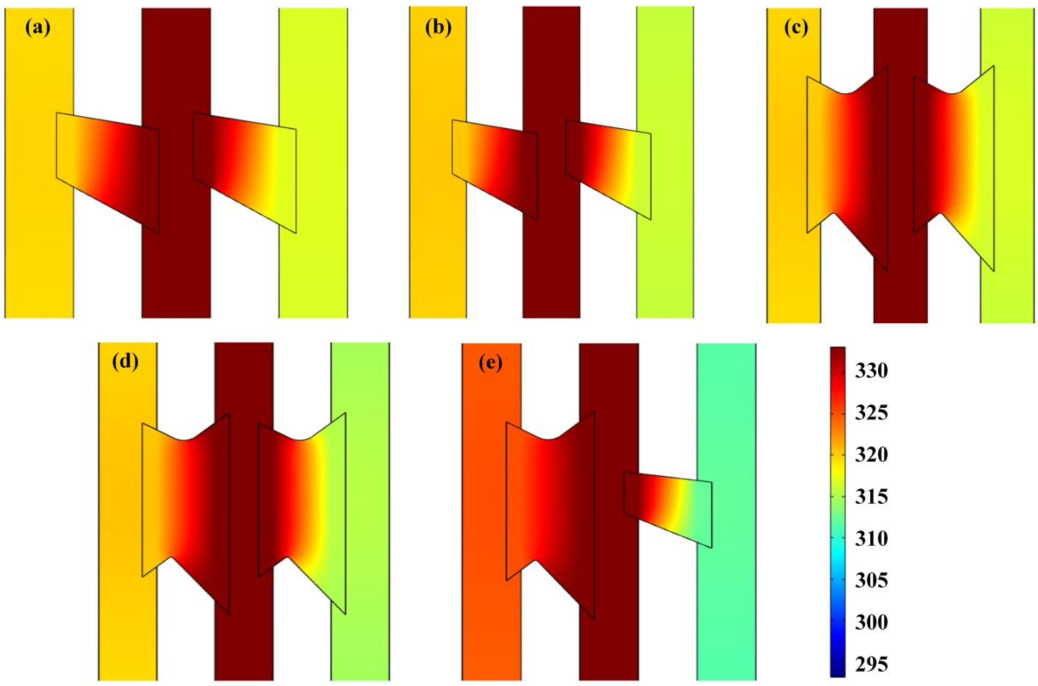

Figure S2. Simulation results of five thermal rectifier

For the thermal analysis of thermal transistor, three group models were conducted as shown in **Figure S3**(a-l). The first group is the 1T phase of sample 2 on the left and the 2H phase of sample 1 on the right. The second group is the 2H phase of sample 2 on the left and the 2H phase of sample 1 on the right. The third group is the 1T phase of sample 1 on the left and the 2H phase of sample 1 on the right. The model structure is like the structure of thermal rectifier. The temperature of the left electrode is a constant value of 323.15K, the temperature of the right electrode is a constant value of 373.15K, and the temperature of the middle electrode is a constant value that changes with time, 303.15K/0~0.2s, 333.15K/0.2~0.3s, 363.15K/0.3~0.4s, 393.15K/0.4~0.5s. The thermal conductivity of MoS_2 samples were also determined according to the experimental value. The heat flow transferred among the cross-plane direction was the only unknown parameter.

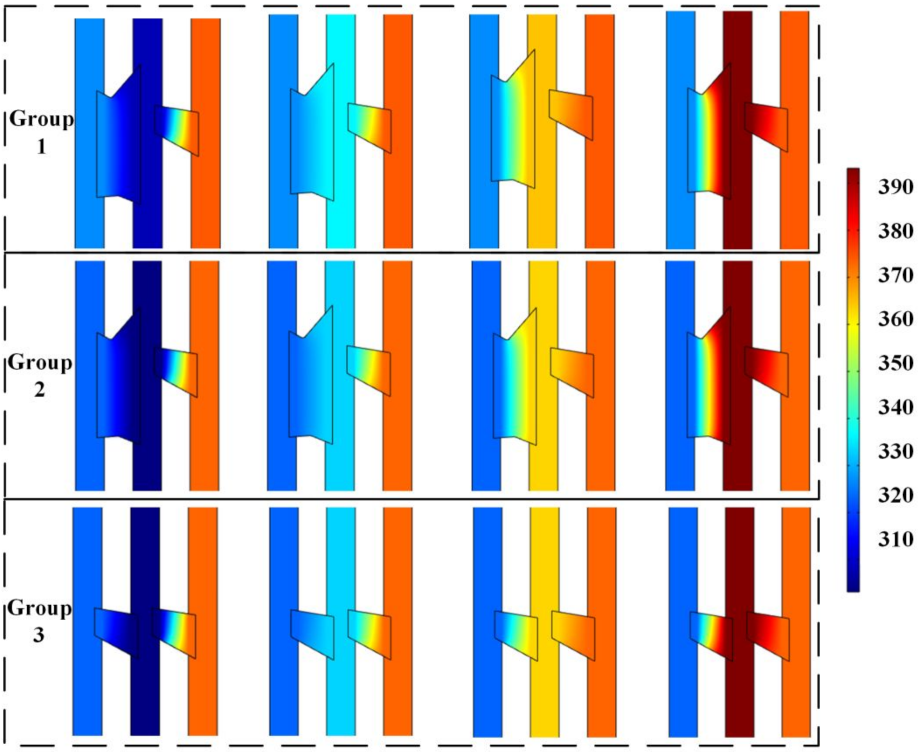

Figure S3. Thermal analysis results of three thermal transistor

6. Uncertainty analysis

According to the error transfer formula, the thermal conductivity error can be calculated with equations below [5].

$$\left(\frac{\delta\lambda}{\lambda}\right)^2=\left(\frac{\delta Q}{Q}\right)^2+\left(\frac{\delta\Delta T}{\Delta T}\right)^2+\left(\frac{\delta A}{A}\right)^2+\left(\frac{\delta L_s}{L_s}\right)^2 \tag{7}$$

$$\left(\frac{\delta Q}{Q}\right)^2=2\left(\frac{\delta U_1}{U_1}\right)^2+\left(\frac{\delta R_1}{R_1}\right)^2+\left(\frac{\delta T_1}{T_1}\right)^2+2\left(\frac{\delta T_2}{T_2}\right)^2 \tag{8}$$

$$\left(\frac{\delta A}{A}\right)^2=\left(\frac{\delta t}{t}\right)^2+\left(\frac{\delta D}{D}\right)^2 \tag{9}$$

$$\left(\frac{\delta\Delta T}{\Delta T}\right)^2=\left(\frac{\delta T_1}{T_1}\right)^2+\left(\frac{\delta T_2}{T_2}\right)^2 \tag{10}$$

$$\left(\frac{\delta T_1}{T_1}\right)^2=\left(\frac{\delta R_1}{R_1}\right)^2+2\left(\frac{\delta R_{01}}{R_{01}}\right)^2,\left(\frac{\delta T_2}{T_2}\right)^2=\left(\frac{\delta R_2}{R_2}\right)^2+2\left(\frac{\delta R_{02}}{R_{02}}\right)^2 \tag{11}$$

$$\left(\frac{\delta\eta}{\eta}\right)^2 = 2\left(\frac{\delta\lambda_p}{\lambda_p}\right)^2 + \left(\frac{\delta\lambda_n}{\lambda_n}\right)^2 \tag{12}$$

The voltage was supplied by a lock-in amplifier (7265 DSP) and the minimum heating voltage was 0.045 V with an uncertainty of 0.001 V. So the the uncertainty of U_1 was $\delta U_1 / U_1$ ~ 2.22%. The resistance was controlled by a resistor box, which was 0.1 ohms of adjustable minimum, and the minimum initial and measuring resistance were 19.1 and 19.8 ohms, so the uncertainty of R_0 and R was $\delta R_0 / R_0$ and $\delta R / R$ ~ 0.52% and 0.51%. Both the length and the width were determined with the SEM image, and the uncertainty of length and width was $\delta L_s / L_s$ and $\delta D / D$ ~ 0.50%. The thickness of ten layers MoS_2 was measured by AFM with an uncertainty of 0.03nm, so the uncertainty of thickness was $\delta t / t$ ~ 0.46%. The temperature rise of the electrode was calculated according to the relationship between resistance and temperature, so the uncertainty of ΔT was $\delta\Delta T / \Delta T$ ~ 0.89%. By substituting all these uncertainties into equations (7) and (12), $\delta\lambda / \lambda$ and $\delta\eta / \eta$ were calculated as ~ 3.85% and 6.66%.

References

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