

1次元原子欠陥トンネルを含む酸化タングステン薄膜の熱電特性

Thermoelectric Properties of Tungsten Oxide Films with 1D Atomic Defect Tunnels

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The coexistence of high electron conduction and low heat conduction is essentially important to realize efficient thermoelectric materials. Although introducing 0D point defects or 2D layers is known as an effective way to reduce the heat conduction, there is a dilemma that the electron conduction is also reduced due to that electrons and phonons are scattered simultaneously by impurities, defects, and boundaries. Here we show that introducing a 1D atomic defect tunnel which is epitaxially stabilized in oxygen deficient tungsten oxide WO_x films is an excellent solution to solve this dilemma.

The WO_x films ($2.7 < x < 3.0$) were heteroepitaxially grown on (001) and (110) LaAlO_3 single crystal substrates by PLD. HAADF-STEM observation revealed that the resultant WO_x epitaxial films contain 1D atomic defect tunnel in the in-plane direction and the density increased with decreasing x . The 1D atomic defect tunnels were formed along [001] with extremely high density.

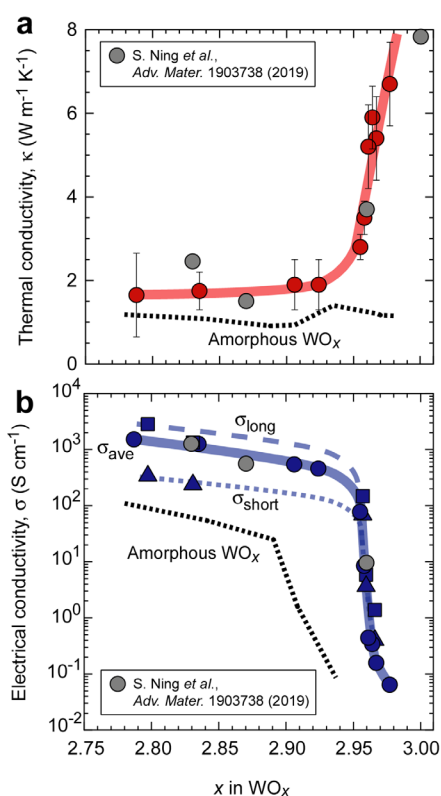
The thermal conductivity (κ) of the films drastically decreased from ~ 7 to $\sim 1.5 \text{ W m}^{-1} \text{ K}^{-1}$ with increasing 1D defects (**Fig. a**). The κ values of WO_x films are closed to that of amorphous WO_x ^[1], which shows minimum κ . The introduction of 1D defect tunnels effectively suppress the phonon propagation.^[2]

On the other hand, the electrical conductivity (σ) in the in-plane direction of WO_x film dramatically increased from $\sim 10^{-1}$ to $\sim 10^3 \text{ S cm}^{-1}$ (**Fig. b**). Since the oxygen removal reduces the valence state of tungsten, carrier electron concentration increases with increasing 1D defects. The σ along the tunnels is 5 times larger than that across the tunnels.^[3]

These results clearly indicate that high electron conduction and low heat conduction coexist in the oxygen-deficient tungsten oxide epitaxial films. The present finding would be useful to design efficient thermoelectric materials.

References

[1] G. Kim *et al.*, *J. Phys. Chem. C* **123**, 15419 (2019). [2] G. Kim *et al.*, *ACS Appl. Electron. Mater.* **2**, 2507 (2020). [3] G. Kim *et al.*, in submission.



(a) Cross-plane thermal conductivity κ extracted from the TDTR measurement. The κ of amorphous WO_x films and epitaxial WO_x films are also plotted. (b) In-plane electrical conductivity σ . The σ of amorphous WO_x films and epitaxial WO_x films are also plotted.