Highlights

Innovative materials with strong interplay of spin orbital charge and topological degrees of freedom - 2018

Intrinsic Origin of Enhancement of Ferroelectricity in SnTe Ultrathin Films

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PHYSICAL REVIEW LETTERS 121 (2018) 027601

Previous studies showed that, as ferroelectric films become thinner, their Curie temperature (Tc) and polarization below Tc both typically decrease. In contrast, a recent experiment [Chang et al., Science 353, 274 /(2016)] observed that atomic-thick SnTe films have a higher Tc than their bulk counterpart, which was attributed to extrinsic effects. We find, using first-principles calculations, that the 0-K energy barrier for the polarization switching (which is a quantity directly related to Tc) is higher in most investigated defect-free SnTe ultrathin films than that in bulk SnTe, and that the 5-unit-cell (UC) SnTe thin film has the largest energy barrier as a result of an interplay between hybridization interactions and Pauli repulsions. Further simulations, employing a presently developed effective Hamiltonian, confirm that freestanding, defect-free SnTe thin films have a higher Tc than bulk SnTe, except for the 1-UC case. Our work, therefore, demonstrates the possibility to intrinsically enhance ferroelectricity of ultrathin films by reducing their thickness.

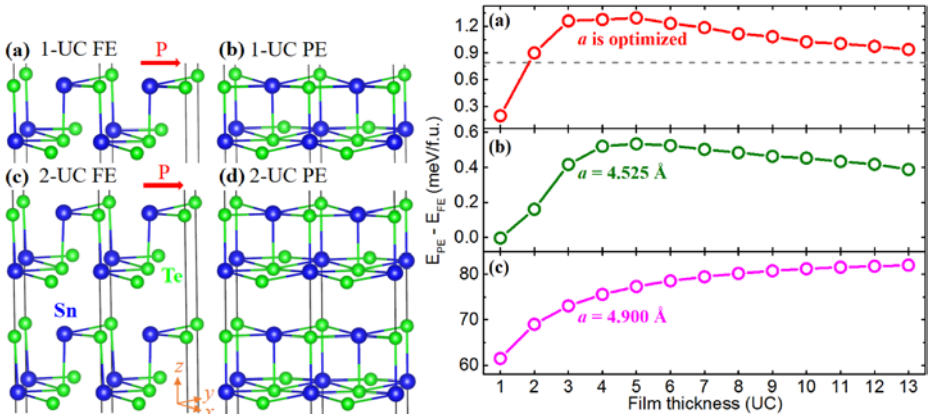

Fig. 1: Left panels: Crystal structures of SnTe thin films. Ferroelectric (FE) phases of (a) 1-UC and (c) 2-UC SnTe thin films. Paraelectric (PE) phases of (b) 1-UC and (d) 2-UC SnTe thin films. The red arrows indicate that polarizations are along the [110] direction. Right panels: Thickness dependence of the energy barriers between the PE and FE phases of SnTe films (a) with fully optimized lattice constants *a* and *b*, (b) when *a* and *b* are fixed at the bulk lattice constant of 4.525 Å, and (c) with a 7.2% tensile strain. The dashed line shows the results for bulk SnTe.