Development of Bi2Te3-based Thermoelectric Thin Films Using Advanced Pulsed Laser Deposition System

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Abstract

This study presents the pulsed laser deposition of n-type selenium (Se)-doped bismuth telluride ($Bi_2Te_{2.7}Se_{0.3}$) and n-type bismuth telluride (Bi_2Te_3) nanostructures at varying substrate temperatures. The effects of substrate temperature on the structural, morphological, and thermoelectric properties of these nanostructures were systematically explored. Density functional theory (DFT) simulations were conducted to examine the electronic structures, partial, and total densities of states of the unit cells of the compounds. Surface and structural characterization revealed highly crystalline nanostructures with pronounced grain boundaries. A comparative analysis underscores the impact of Se inclusion on the thermoelectric performance of the Bi_2Te_3 matrix. The study also highlights the substrate temperature-dependent variations in the thermoelectric figure of merit (ZT). Notably, the room temperature thermoelectric power factors (PF) of 2765 $\mu W/mK^2$ for pure Bi_2Te_3 and 3179 $\mu W/mK^2$ for Se-doped Bi_2Te_3 demonstrate their promise for cooling and power generation applications. The Se-doped Bi_2Te_3 exhibited a room temperature ZT value of 0.92, representing a 30% improvement over the pure phase. This enhancement is attributed to the reduction in thermal conductivity due to increased phonon scattering at the interfaces in the doped material.