

Single-crystalline Bismuth Telluride Nanowires for High-efficiency Thermoelectric Devices

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High efficient thermoelectricity requires materials with a large figure of merit, ZT , defined as $ZT = \sigma S^2 T / \kappa$, where σ is the electrical conductivity, S the thermoelectric power, and κ the thermal conductivity. However, due to the interdependence of σ , S , and κ , the optimization of thermoelectric properties remains challenging. It is well known that there are two approaches to enhanced ZT values. One is to utilize quantum confinement effects of nanostructures, providing an opportunity to individually control σ and S , and thus to promote ZT because of the increase of the density of states (DOS) [1]. The other is to reduce κ without having an effect on σ and S by using semiconductors of high atomic weight such as bismuth telluride (Bi_2Te_3) with much lower atomic vibration frequencies [2].

In this work, we present a new method to grow high-quality, single-crystalline Bi_2Te_3 nanowires, which can be used in thermoelectric devices with high thermoelectric figure-of-merit ZT values. $\text{Bi}_x\text{Te}_{1-x}$ ($x=0.35\sim 0.55$) thin films were grown on an thermally oxidized Si substrate by an UHV sputtering system with a Bi (99.999%) and a Te target (99.99%). For the growth of $\text{Bi}_x\text{Te}_{1-x}$ nanowires, the co-sputtered films were transferred to a furnace for thermal annealing in the temperature range 300-450°C. Interestingly, uniform and straight Bi_2Te_3 nanowires with high aspect ratios were found to grow on the surface of the co-sputtered films after annealing. The growth of the Bi_2Te_3 nanowires is attributable to their relaxation of stress, originating from a thermal expansion mismatch between the film and the substrate. This mismatch is due to the large difference in the coefficient of thermal expansion of $\text{Bi}_x\text{Te}_{1-x}$ ($\sim 19 \times 10^{-6}/^\circ\text{C}$), SiO_2 ($0.5 \times 10^{-6}/^\circ\text{C}$) and Si ($2.4 \times 10^{-6}/^\circ\text{C}$).

A high-resolution TEM study reveals that the Bi_2Te_3 nanowire with $d = 65$ nm grown along the $\langle 110 \rangle$ direction is high-quality single crystalline. The diffraction pattern recorded perpendicular to the long axis of the nanowire can be indexed to the hexagonal lattice of Bi_2Te_3 ($a=4.385\text{\AA}$, $c=30.483\text{\AA}$) with [001] zone axis. The Bi_2Te_3 nanowires were found to have diameters ranging from 50 nm to 500 nm depending on the thickness of the co-sputtered $\text{Bi}_x\text{Te}_{1-x}$ films, indicating that the diameter of Bi_2Te_3 nanowires can be tuned by controlling sputtering conditions. Elemental mapping profiles demonstrate that the uniform distribution of Bi and Te along the length of the nanowire without appreciable segregation and the Bi_2Te_3 nanowire with Bi (blue, 40.06%) and Te (red, 59.36%) concentrations. Quantitative analysis of composition variation by line profiles also demonstrates that the Bi and Te are homogeneously distributed through the nanowire. The composition of $\text{Bi}_x\text{Te}_{1-x}$ nanowires were found to be adjusted by tailoring the composition of co-sputtered films from $x = 0.35$ to 0.55.

Our results demonstrate that single-crystalline Bi_2Te_3 nanowires can be grown by a novel stress-induced method, providing a motivation for exploring the high-efficiency thermoelectric properties of single-crystalline Bi_2Te_3 nanowires. Further details on the mechanism of the single-crystalline Bi_2Te_3 nanowires will be presented.

[1] Q. Wei and C.M. Lieber, *Mat. Res. Soc.* 581, 219 (2000).

[2] A. Majumdar, *Science* 303, 777 (2004).