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Influence of surface states and size effects on the Seebeck coefficient and electrical resistance of Bi_{1-x}Sb_x nanowire arrays

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Seebeck coefficient and electrical resistance of $B_{1,x}Sb_x$ nanowire arrays electrodeposited in etched ion-track membranes have been investigated as a function of wire diameter (40 - 750 nm) and composition ($0 \le x \le 1$). The experimental data reveal a non-monotonic dependence between thermopower and wire diameter for three different compositions. Thus, the thermopower values decrease with decreasing wire diameter, exhibiting a minimum around ~ 60 nm. This non-monotonic dependence of the Seebeck coefficient is attributed to the interplay of surface and bulk states. On the one hand, the metallic properties of the surface states can contribute to decrease the thermopower of the nanostructure with increasing surface-to-volume ratio. On the other hand, for wires thinner than ~60 nm, an increase of the thermopower can be attributed to an hybridization of the surface states as well as to quantum size-effects. These measurements contribute to a better understanding of the interplay between bulk and surface states in nanostructures, and indicate an enhancement of the Seebeck coefficient for thinner nanowires.

Electronic supplementary informations:

Influence of surface states and size effects on the Seebeck coefficient and electrical resistance of Bi_{1-x}Sb_x nanowire arrays M. Cassinelli, S. Müller, K.-O. Voss, C. Trautmann, F. Völklein, J. Gooth, K. Nielsch, and M.E. Toimil-Molares.

Seebeck coefficient of ${\sf Bi}_{0.85}{\sf Sb}_{0.15}$ and Sb nanowire arrays as a function of the wire diameter

Fig. ESI 1 reports the evaluated thermopower of (a) $Bi_{0.85}Sb_{0.15}$ and (b) Sb nanowire arrays within the temperature range 300 and 30 K and for wire diameters between ~ 753 nm and ~ 41 nm. Both curves show a monotonous decrease of the Seebeck coefficient as a function of the temperatures, as in case of Bi nanowires measurements (see fig. 3a). The Seebeck coefficients of $Bi_{0.85}Sb_{0.15}$ nanowires are negative considered the wire diameter, due to the ntype character of $Bi_{1-x}Sb_x$ with low Sb concentrations.^{91,92} Sb nanowire arrays possess positive values of the thermopower, as expected for p-type Sb material.⁹³

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Fig. ESI 1 Seebeck coefficient of (a) $Bi_{0.85}Sb_{0.15}$ and (b) Sb nanowire arrays with different wire diameter as a function of temperature. The different wire diameters are: 753 ± 37 (black), 431 ± 29 (red), 130 ± 10 (light green), 113 ± 11 (blue), 79 ± 8 (magenta), 58 ± 6 (brown), 48 ± 7 (green), and 41 ± 5 (orange).

Electrical resistance of ${\rm Bi}_{0.85}{\rm Sb}_{0.15}$ and Sb nanowire arrays as decreasing wire diameter and temperature

Fig. ESI2 reports the normalized value of the electrical resistance (R/R(300 K)) of Bi_{0.85}Sb_{0.15} nanowires as a function of temperature for wire diameter between ~ 753 nm and ~ 40 nm. Compared to the electrical resistance of Sb nanowires (see fig. 5b) the resistance ratio of the alloy is smaller was detected. This is due to the larger charge carrier mean free path of Bi_{1-x}Sb_x alloy than pure Sb which limits the gain of the carrier mobility with decreasing temperature .^{94,95} This effect is more pronounced in wires with smaller diameters, namely 48 ± 7 and 41 ± 5 nm, where the resistivity ratio shows a rather weak dependence on the temperature, varying from ~ 1.0 at 300 K to ~ 0.9 at 30 K.



Fig. ESI 2 Normalized electrical resistance of arrays of $Bi_{0.85}Sb_{0.15}$ wires with average diameter 753 ± 37 (black), 431 ± 29 (red), 130 ± 10 (light green), 113 ± 11 (blue), 79 ± 8 (magenta), 58 ± 6 (brown), 48 ± 7 (green) and 41 ± 5 (orange), as a function of temperature.

Seebeck coefficient of $Bi_{1,x}Sb_x$ alloy nanowires as a function of composition and temperature

Fig. ESI3 shows the evaluated thermopower of $Bi_{1-x}Sb_x$ nanowire arrays (wire diameter 79 nm) for various Sb concentrations as a function of temperature. With decreasing temperature, the thermopower monotonically decreases. The values of the Seebeck coefficient properties were detected only in pure Sb nanowire arrays indicate p-type properties, whereas $Bi_{1-x}Sb_x$ nanowire arrays are n-type material within $0 \le x \le 0.33$.



Fig. ESI 3 Experimental evaluated Seebeck coefficient as a function of temperature for $Bi_{1:x}Sb_x$ alloy nanowire arrays with wire diameter of 79 ± 8 nm. The wires have a composition x(Sb): 0 (black), 0.10 (red), 0.12 (green), 0.18 (blue), 0.33 (magenta), 1 (purple).

Notes and references to ESI

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