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Electronic band structure calculations of bismuth-antimony nanowires ANDREI LEVIN, Harvard University, MILDRED DRESSELHAUS, Massachusetts Institute of Technology — Alloys of bismuth and antimony received initial interest due to their unmatched low-temperature thermoelectric performance, and have drawn more recent attention as the first 3D topological insulators. One-dimensional bismuth-antimony (BiSb) nanowires display interesting quantum confinement effects, and are expected to exhibit even better thermoelectric properties than bulk BiSb. Due to the small, anisotropic carrier effective masses, the electronic properties of BiSb nanowires show great sensitivity to nanowire diameter, crystalline orientation, and alloy composition. We develop a theoretical model for calculating the band structure of BiSb nanowires. For a given crystalline orientation, BiSb nanowires can be in the semimetallic, direct semiconducting, or indirect semiconducting phase, depending on nanowire diameter and alloy composition. These “phase diagrams” turn out to be remarkably similar among the different orientations, which is surprising in light of the anisotropy of the bulk BiSb Fermi surface. We predict a novel direct semiconducting phase for nanowires with diameter less than ~ 15 nm, over a narrow composition range. We also find that, in contrast to the bulk and thin film BiSb cases, a gapless state with Dirac dispersion cannot be realized in BiSb nanowires.

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