Bismuth Nanobelts for Enhanced Thermoelectric Performance\textsuperscript{1}

XU ZHAO, MING TANG, GANG CHEN, M. S. DRESSELHAUS, Massachusetts Institute of Technology, Cambridge, MA, ZHIFENG REN, Boston College, Chestnut Hill, MA — Bismuth is a semimetal with high promise for thermoelectric applications if it could be made into a semiconductor by a combination of size reduction (based on quantum confinement considerations) and antimony addition. The recent experimental preparation of bismuth Nanobelts has motivated calculation of the phase diagram for the bismuth-antimony system in the regime of nanobelt cross sectional area and antimony concentration where semiconducting behavior is expected. Both direct and indirect bandgap regions are considered and regimes where the highest valence band is at the T-point, the L-point and the H-point are identified. The dependence of the semiconductor-semimetal transition on sample geometry, crystal orientation and temperature will be considered to guide in the preparation of a sample set for use in exploration of this materials system for thermoelectric applications.

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