Effect of nano-crystallization and atomic substitution on electronic and heat properties of Bi2Te3

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**Abstract**. The specific heat of nano-crystalline (NC) Bi2Te3 (20 nm) in the temperature range of 150 K to 300 K is theoretically studied and compared with the specific heat of the bulk Bi2Te3 materials. Carrier concentration and Hall coefficient also evaluated using free electron model and compared with experimental results. Theoretically, the specific heat of nanocrystalline (NC) Bi2Te3 (20nm) in the given temperature range is evaluated. Lattice (phonon) specific heat has been observed with an overlap repulsive potential with the help of Debye model. For Nano Crystalline materials having high interface volume ratio, the Debye temperature and phonon frequencies are reasonably less at the interfaces than at the core of nano-crystal. Such softening of phonon frequencies at interfaces results in enhancement of Specific Heat in nano-structures. Total specific heat would include interface, core and electronic specific heat. The temperature derivative of the internal energy yields the electronic contribution to specific heat. The present analysis based on the softening of phonon frequencies mechanism is sufficient to describe the enhancement in specific heat by nano-crystallization.