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Effect of Spin-Orbit Interaction on the Lattice Properties of Solids: Sb and Bi M. CARDONA, MPI fuer Festkoerperforschung, D-70569 Stuttgart, Germany, L. E. DIAZ-SANCHEZ, CINVESTAV-Queretaro, 76230 Queretaro, Qro., Mexico, X. GONZE, Unite de Physico-Chimie et de Physique des Materiaux, Universite Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium , R. K. KREMER, MPI fuer Festkoerperforschung, D-70569 Stuttgart, Germany, A. H. ROMERO, CINVESTAV-Queretaro, 76230 Queretaro, Qro., Mexico, J. SERRANO, ICREA, EPSC Universitat Politecnica de Catalunya, 08860 Castelldefels, Spain — We present measurements of the specific heat (C) vs. $T$for Bi and Sb and vs. isotopic mass for Sb. The measurements are compared with *ab-initio* calculations performed with the ABINIT code, including spin-orbit (S-O) interaction. It is shown that the S-O interaction softens the lattice and thus increases the value of Cat the low Tmaximum (T_m ∼8K for Bi, T_m ∼14K for Sb), improving agreement between theory and experiment. The effect of S-O interaction on other thermodynamic properties, such as the lattice parameter, a_0, and the cohesive energy, E_c, is also calculated. It is shown that this interaction decreases E_c and, correspondingly, increases a_0. These effects are proportional to $c_2\lambda^{\ 2} + c_3\lambda^3$, where λ is the S-O coupling constant, about twice as large for Bi as for Sb.

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