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 \textit{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 \( C \) at the low \( T \) maximum \( (T_m \sim 8K \) for Bi, \( T_m \sim 14K \) 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 \( \lambda \) is the S-O coupling constant, about twice as large for Bi as for Sb.

M. Cardona
MPI fuer Festkoerperforschung, D-70569 Stuttgart,