Characterization and decomposition of the natural van der Waals heterostructure $SnSb_2Te_4$ under compression

J. A. Sans,[1,*] R. Vilaplana,[2] E. L. Da Silva,[1] C. Popescu,[3] V. P. Cuenca-Gotor,[1] A. Andrada-Chacón,[4] J. Sánchez-Benitez,[4] O. Gomis,[2] A. L. J. Pereira,[1,5] P. Rodríguez-Hernández,[6] A. Muñoz,[6] D. Daisenberger,[7] B. García-Domene,[8] A. Segura,[8] D. Errandonea,[8] R. S. Kumar,[9] O. Oeckler,[10] J. Contreras-García,[11] and F. J. Manjón[1]

[1] *Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team, Universitat Politècnica de València, Valencia, Spain*
[2] *Centro de Tecnologías Físicas, MALTA-Consolider Team, Universitat Politècnica de València, Valencia, Spain*
[3] *ALBA-CELLS, Barcelona, Spain*
[4] *Departamento de Química-Física, MALTA-Consolider Team, Universidad Complutense de Madrid, Madrid, Spain*
[5] *Grupo de Pesquisa de Materiais Fotonicos e Energia Renovavel - MaFER, Universidade Federal da Grande Dourados, Dourados, Brazil*
[6] *Departamento de Física, MALTA-Consolider Team, Instituto de Materiales y Nanotecnología, Universidad de La Laguna, Tenerife, Spain*
[7] *Diamond Light Source Ltd, Oxon, England*
[8] *HP Science and Engineering Center, Department of Physics and Astronomy, University of Nevada Las Vegas, 4505 Maryland Parkway, Las Vegas, Nevada, USA*
[9] *Institut für Mineralogie, Kristallographie und Materialwissenschaft, Universität Leipzig, Germany*
[10] *CNRS, UMR 7616, Laboratoire de Chimie Théorique, Paris, France*
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*e-mail: juasant2@upv.es

The observation of 3D-topological insulators (TIs) in A_2X_3 binary compounds with layered tetradymite structure **[1]**, has triggered the exploration of layered ternary BA_2X_4 compounds based on those A_2X_3 binary compounds in order to look for 3D-TI properties with a richer physics **[2]**. Noteworthy, electronic band structure calculations have predicted 3D-TI behavior in many layered ternary BA_2X_4 compounds, like rhombohedral $SnSb_2Te_4$ with layered tetradymite-like structure **[3]**.

Here, we present a joint experimental and theoretical study of the structural, vibrational and electrical properties of rhombohedral $SnSb_2Te_4$ at high pressure, which unveils the internal mechanisms developed during its compression. The equation of state and the internal polyhedral compressibility, the symmetry and behavior of the Raman-active modes and the electrical behavior of this 3D-TI under compression have been discussed and compared to its parent binary Sb_2Te_3 and SnTe compounds and other related ternary compounds.

Our X-ray diffraction and Raman measurements together with theoretical calculations, which include topological electronic analysis, evidence the presence of an isostructural phase transition above 2.5 GPa and a Fermi resonance around 3.5 GPa. Moreover, the analysis of the electrical properties can be explained by the creation of defects along the ongoing isostructural phase transition.

The analysis of the frequency of the Raman-active modes and their evolution under pressure of $SnSb_2Te_4$ reveals a strong correlation with the vibrational modes of its parent binary compounds. This makes possible to identify the HP evolution of the Raman-active modes of α-Sb_2Te_3 and even the Raman-inactive LO-mode of c-SnTe. Consequently, we propose that Raman spectroscopy of ternary compounds can be a useful tool to unveil Raman-inactive modes of their binary constituents.

Above 7 GPa, $SnSb_2Te_4$ exhibits a pressure-induced decomposition into the high-pressure phases of its parent binary compounds. This behavior is framed within the orbital radii map of BA_2Te_4 compounds, whose extension paves the way to understand the pressure behavior and stability ranges of other layered van der Waals-type compounds with similar stoichiometry.

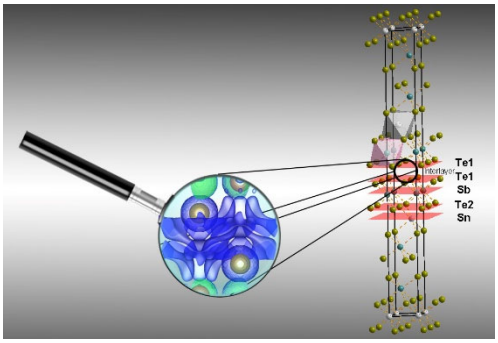

Figure 1. Detail of the analysis of the interlayer interactions in rhombohedral $SnSb_2Te_4$

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