Structural, Vibrational, and Electronic Behavior of Two GaGeTe Polymorphs under compression.

E. Bandiello[1,*], S. Gallego-Parra[1,*], A. Liang,[2] J.A. Sans[1], V. Cuenca-Gotor[1], E. Lora da Silva[3], R. Vilaplana[4], P. Rodríguez-Hernández[5], A. Muñoz[5], D. Diaz-Anichtchenko[2], C. Popescu[6], F.G. Alabarse[7], C. Rudamas[8], C. Drasar[9], A. Segura[2], D. Errandonea[2], and F.J. Manjón[1]

[1] *Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team, Universitat Politècnica de València, 46022 Valencia, Spain*
[2] *Departamento de Física Aplicada-ICMUV, MALTA Consolider Team, Universitat de València, 46100 Burjassot, Spain*
[3] *IFIMUP, Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Department of Physics and Astronomy, Faculty of Sciences, University of Porto, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal*
[4] *Centro de Tecnologías Físicas, MALTA Consolider Team, Universitat Politècnica de València, 46022 València, Spain*
[5] *Departamento de Física, Instituto de Materiales y Nanotecnología, MALTA Consolider Team, Universidad de La Laguna, La Laguna, 38205 Tenerife, Spain*
[6] *CELLS-ALBA Synchrotron Light Facility, MALTA Consolider Team, 08290 Cerdanyola del Vallès, Barcelona, Spain*
[7] *Elettra Sincrotrone Trieste, S.S. 14 - km 163,5 in AREA Science Park, 34149 Basovizza, Trieste, Italy*
[8] *Escuela de Física, Facultad de Ciencias Naturales y Matemática, Universidad de El Salvador, San Salvador, El Salvador*
[9] *Faculty of Chemical Technology, University of Pardubice, Pardubice 532 10, Czech Republic*

Abstract

GaGeTe is a layered topological semimetal that has been recently found to exist in at least two different polytypes, α-GaGeTe ($R\bar{3}m$) and β-GaGeTe ($P6_3mc$). Here we report a joint experimental and theoretical study of the structural, vibrational, and electronic properties of these two polytypes at high pressure. Both polytypes show anisotropic compressibility and two phase transitions, above 7 and 15 GPa, respectively, as confirmed by XRD and Raman spectroscopy measurements. Although the nature of the high-pressure phases could not be confirmed, possible high-pressure phases for both polytypes, with an increase in coordination for Ga and Ge atoms from 4 to 6, have been proposed by comparison with other chalcogenides and total-energy calculations. The simplification of the X-ray pattern for both polytypes above 15 GPa suggests a transition to a structure of relatively higher symmetry than the original one. This result is consistent with the rocksalt-like high-pressure phases observed in parent III-VI semiconductors, such as GaTe, GaSe, and InSe. Pressure-induced amorphization is observed upon pressure release. The electronic band structures of α-GaGeTe and β-GaGeTe and their pressure dependence also show similarities to III-VI semiconductors, thus suggesting that the germanene-like sublayer induces a semimetallic character in both GaGeTe polytypes. Above 3 GPa, both polytypes lose their topological features, due to the opening of the direct band gap.

Keywords: GaGeTe, phase transition, XRD, Raman, band gap.