Journal of Acoustical Engineering Society of Iran, Vol. 8, No. 2, 2021

(Research Article)
Ab-initio calculation of elastic, mechanical and acoustic properties of BeX (X= S, Se, Te) compounds

H. Salehi*, P. Amiri, F. Hashemi
Department of Physics, Faculty of Science, Shahid Chamran University of Ahvaz

Abstract

In this paper the elastic, mechanical (stability, anisotropy and Poisson's coefficients) and acoustic properties of BeX (X= S, Se, Te) have been investigated. Calculations with Full potential linear augmented plane wave have been performed in the framework of density functional theory with LDA, PBE-GGA and MBJ approximations by using Wien2k computational package. Elastic properties such as, elastic constants, Shear modulus, Young modulus and Debye temperature were calculated within various approximations for cubic and hexagonal structural phases. The calculated elastic properties indicate the give rise to an elastic stability and anisotropy property of the compounds. The results also indicate that these compounds are more brittle in the cubic phase and more malleable in the hexagonal phase. In fact, the ductility of these compounds in the cubic structural phase is low and they can be placed in the category of non-formable materials.

Keywords: Density functional theory, Acoustic properties, Elastic properties, Elastic stability.

pp. 96-103 (In Persian)

* Corresponding author E-mail: salehi_h@scu.ac.ir

[DOR: 20.1001.1.23455748.1399.8.2.10.7]