Abstract

A comprehensive theoretical analysis exploring the effect of metal doping (Mg, Ca, and Sr) on phase transition, electronic band structure and their repercussions on the optical, elastic, and mechanical properties of $BaThO_3$ has been presented. This analysis was carried out in order to learn more about these properties. The structure of $BaThO_3$ stays cubic even when doped with 1.40 % of Mg, Ca, and Sr-atoms; however, when the doping concentration is increased to 4.22% or 7.04%, the structure transitions from cubic to a pseudo-cubic tetragonal phase is noted. In every instance of doping, a systematic and noticeably large narrowing of the band gap is seen and the nature of this phenomenon is shown to be directly related to the G-symmetry point. The total density of states (TDOS), partial density of states (PDOS), and elemental partial density of states (EPDOS) are in line to understand the narrowing of the band gap. The optical response of the doped material displays a red shift in the absorption edge, whilst the refractive index rises from 2.067-2.227 with Mg-doping and marginally lowers with Ca and Sr doping. The estimated elastic constants for cubic and tetragonal symmetry follow the mechanical stability criterion for each doping concentration, with the exception of 7.04%Ca doping, which deviates from this rule. In addition, when elastic parameters are used, the bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio, and anisotropic anisotropy (A) are computed as estimates. In order to evaluate the brittleness or ductility of a pure or doped compound, the B/G value must first be calculated. In addition, non-homogeneity is shown when doping levels are 4.22%Ca, 7.04%Ca and 4.22%Mg. This is because the negative stiffness and extremely high Poisson ratio values cause the problem. Doping a compound with calcium, magnesium, or strontium would cause changes in its electronic structure, optical, and mechanical properties. Due to the fact that the doped compound absorbs in the UV range, these changes would make it a good candidate for better optimization as a UV filter.