DFT calculation for elastic constants of orthorhombicstructure within WIEN2K code: A new package (ortho-elastic)

Abstract

A new package for calculating the elastic constants of orthorhombic structure is released. The package called ortho-elastic. The formalism of calculating the ortho-elastic constants is described in details. The package is compatible with the highly accurate all-electron full-potential (linearized) augmented plane-wave plus local orbital [FP-(L)APW+lo] method implemented inWIEN2k code. Several orthorhombic structure compounds were used to test the new package. We found that the calculated elastic constants using the new package show better agreement with the available experimental data than the previous theoretical results used different methods. In this package the second-order derivative $E''()$ of polynomial fit $E=E()$ of energy vs strains at zero strain ($=0$), used to calculate the orthorhombic elastic constants.