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IRelast package

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ABSTRACT

In this paper, we present the effectiveness of the IRelast package for the elastic constants (ECs) of crystals with different symmetries like Cubic, Hexagonal, Tetragonal, Orthorhombic, Rhombohedral and Monoclinic which are further used to investigate elastic and mechanical properties. The calculated results confirm the usefulness of the software by reproducing consistent experimental results. The reason for this competency is energy approach, where the calculated total ground state energy $E(y, \varepsilon_{ij})$ is used for the calculations of the ECs. The software is also incorporated into the WIEN2K package. The purpose of the software is to provide a theoretical tool for researchers to calculate ECs of the unknown compounds and calculate ECs for experimentally measured ones for comparison purpose.

1. Introduction

The elastic properties of materials are crucial for their engineering, scientific and medical applications such as the elastic strength of pillars and beams in buildings and bridges, compatibility of medical and dental materials with the tissues and bones of human body and strong but light materials for planes and automobiles. Hence, elastic properties are essential for the applications of materials and they can be easily evaluated by using the elastic constants. Density functional theory (DFT) is a very successful theoretical tool for the calculation of elastic constants of solids.

DFT has emerged as a very powerful technique for solving many body problem using Kohn–Sham (KS) equations [1–4]. Exchange-correlation functional poses a question mark on the precision of DFT as its exact form is unknown [5]. Therefore, selection of exchange–correlation functional is of great importance in DFT. Different approximations are used for exchange–correlation functional to reach accurate results [6–11]. The accuracy of DFT can be seen from the statistics that of the top three most cited physicists, the first (Perdew: 65757 citations) and third (Becke: 62581 citations) are density-functional theorists [12]. The top three most cited physics papers, and eight of the top ten, are in the field of DFT [13,14]. DFT is used to calculate many physical and chemical properties of solids and one of them is elastic compliance constants or simply elastic constants (ECs).

Elastic constants play key role in defining materials properties and show their response when exposed to the external forces [15–18]. Elastic constants provide a connection between the atomic and the large-scale world [19–21]. Therefore, the validity of microscopic and macroscopic theories can be tested by comparing evaluated ECs with the experimental results. Using the elastic stability criteria, ECs can be used to differentiate elastic from plastic regimes [20,22,23]. Different physical properties like hardness, Voigt's modulus, Reuss's modulus, Hill's modulus, shear modulus, Young's modulus, bulk modulus, elastic stiffness coefficients, Poisson's ratio, and melting temperature are calculated using ECs [24]. Similarly, phonon dispersion spectrum, entropy, thermal expansion coefficient, and other thermodynamic properties are related to the ECs as well [25–27]. Sound velocities in different directions and as a result Debye temperature are also calculated by

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the ECs [28,29]. Moreover, ECs are also used to calculate elastic anisotropy ratio, which explains phase stability of crystal structures [30].

Since many of the DFT codes do not have facilities for the elastic constants of different types of crystals, therefore in this article we discuss the effectiveness of our in-house software, IRelast package, developed by M. Jamal. The article discusses the use and effectiveness of the software for different symmetries of crystals. The software is already integrated in 2014 to the WIEN2K, which is one of the most commonly used DFT codes. The IRelast package effectively calculates elastic properties of crystals with different symmetries based on the second order derivative of energy vs. strain at zero-strain.

2. Theoretical background

Elastic constants, which distinguish elastic from plastic regimes, are derived using two different methods. One method is called energy approach discussed by Stadler [31] in which calculated total ground state energy $E(y, \varepsilon_{ij})$, is used for calculating ECs. Nielsen and Martin [32] propose another method called stress theorem in which relation between σ_{ij} and ε_{ij} or vice versa is used for calculation of ECs. Here y represents volume V of the material under pressure (strain) while σ_{ij} and ε_{ij} represent elements of stress and strain respectively [24]. We used the first method to implement IRelast package. Consequently, we used IRelast package as interfaced to the WIEN2k code [33] within the *ab initio* FP-(L)APW + lo method [34] to calculate the elastic constants of different symmetries. For calculation of ECs, we need appropriate strains for different symmetries which are not proposed by energy approach therefore, we try to use suitable strains for each symmetry. Naturally, these strains put a big question mark on the accuracy of the calculated elastic constants therefore; we compared our results with the experimental results in last section. The comparison shows that the results of IRelast package based on the energy approach are in very good agreement with experimental data for different symmetries.

Energy of strained system by a Tailor series expansion for small distortion in the regime of Hooke's law can be written as:

$$E(V, \varepsilon_k) = E_0 + V_0 \left(\sum_{i=1}^{6} \sigma_i \varepsilon_i + \frac{1}{2} \sum_{i,j=1}^{6} C_{ij} \varepsilon_i \varepsilon_j \right) \tag{1}$$

where ε_k represent $\varepsilon_1, \varepsilon_2, \ldots \varepsilon_6$, $E(E_0)$ is the energy and $V(V_0)$ is the volume of strained (unstrained or reference) system. If the strain causes no changes in the volume of the optimized crystal the linear terms vanish because our crystal in equilibrium condition is free of strain. According to the above equation elastic constants (C_{ij}) or linear terms of elastic constants (for example C_{11}-C_{12} or C_{11}+2C_{12}) can be derived by using the second order derivative of equation (1) at zero-strain:

$$C_{ij} = \frac{1}{V_0} \left[\frac{\partial^2 E}{\partial \varepsilon_i \partial \varepsilon_j} \right]_{\varepsilon_k = 0} \tag{2}$$

The above method which calculates elastic constants using the calculated total ground state energy of the distorted system known as the energy approach discussed by Stadler et al. [31] and Wen et al. [35].

If we imagine the bravais lattice vectors of reference structure as a matrix form R the distortion of the lattice R' is represented by multiplying R with a symmetric $(\varepsilon_{xy} = \varepsilon_{yx})$ distortion matrix, i.e. $R' = R \times D$ which is written as,

$$D = I + \varepsilon = \begin{pmatrix} 1 + \varepsilon_{xx} & \frac{\varepsilon_{xy}}{2} & \frac{\varepsilon_{xz}}{2} \\ \frac{\varepsilon_{yx}}{2} & 1 + \varepsilon_{yy} & \frac{\varepsilon_{yz}}{2} \\ \frac{\varepsilon_{zx}}{2} & \frac{\varepsilon_{zy}}{2} & 1 + \varepsilon_{zz} \end{pmatrix} \tag{3}$$

where I is unique matrix and ε represents the symmetric strain tensor. x,y and z are Cartesian indices. In order to reduce the number of indices, it is often convenient to change to the Voigt notation as in Voigt notation we convert xx→1, yy→2, zz→3, zy (and yz)→4, xz (and zx)→5, xy (and yx)→6,

$$D = \begin{pmatrix} 1 + \varepsilon_1 & \frac{\varepsilon_6}{2} & \frac{\varepsilon_5}{2} \\ \frac{\varepsilon_6}{2} & 1 + \varepsilon_2 & \frac{\varepsilon_4}{2} \\ \frac{\varepsilon_5}{2} & \frac{\varepsilon_4}{2} & 1 + \varepsilon_3 \end{pmatrix} \tag{4}$$

Since different symmetries have different independent elastic constants, we need different strains to determine these elastic constants. These different strains based on the Voigt notation along with the second order derivative of energy vs. strain at zero-strain have been presented in the following table.

ECs are used to calculate different mechanical properties. Shear modulus, S_H, as per Hill's average [36] consists of Voigt, S_V and Reuss, S_R [37] values which are calculated using ECs. Shear modulus is measure of resistance to reversible deformation upon shear stress [38] and following equations describe S_V, S_R and S_H.

$$S_V = \frac{1}{5}[(C_{11} + C_{22} + C_{33}) - (C_{12} + C_{13} + C_{23}) + 3(C_{44} + C_{55} + C_{66})] \tag{5}$$

$$S_R = 15[4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{13} + S_{23}) + 3(S_{44} + S_{55} + S_{66})]^{-1} \tag{6}$$

$$S_H = \frac{1}{2}(S_V + S_R) \tag{7}$$

where C_{ij} and S_{ij} denote the elastic constants and elastic compliances, respectively. Similarly, Bulk modulus, B, which shows the response of a material to the uniform hydrostatic pressure, can be calculated from the following equations:

$$B_V = \frac{1}{9}[(C_{11} + C_{22} + C_{33}) + 2(C_{12} + C_{13} + C_{23})] \tag{8}$$

$$B_R = [(S_{11} + S_{22} + S_{33}) + 2(S_{12} + S_{13} + S_{23})]^{-1} \tag{9}$$

$$B_H = \frac{1}{2}(B_V + B_R) \tag{10}$$

The ratio of bulk modulus to shear modulus (B/S) can be used to analyze the ductile or brittle behavior of a material [39]. If B/S ratio is greater than 1.75, then the material will be considered as a ductile otherwise it will be of brittle nature. Using Bulk modulus and shear modulus, we can calculate Young's modulus and Poisson's ratio as per following equations:

$$E = \frac{9BS}{3B + S} \tag{11}$$