# Structural studies of cubic crystals: DFT approach

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**Abstract: Flexibility of materials is involved in determining the load carrying ability and the strength to withstand the exerted load without any deformation. The necessity to understand the physical properties of material becomes an urgent urge to know the fracturing limits of materials for the structural engineering. The current study is aimed to describe the elastic constants for isotropic materials by the relationship between the impose stress and the strain produce within the elastic limit are investigated for certain prescribed materials. The calculation follows the ab initio methodology as a tool for determining the 2nd-order and higher-order elastic constants based on the principle of Density Functional Theory (DFT) which follows on the combination of quantum mechanics with computational techniques. We establish Quantum ESPRESSO as tool for investigating the 2nd-order elastic constants implemented by two approaches based on basic numerical differentiation of the ground energy and the functionals of stress-strain relation by selective codes.**

**Keywords: DFT, Quantum Espresso, Bulk Modulus**

## 1. INTRODUCTION

The mechanical and thermodynamic behavior of materials is a critical field of study within both science and technology. These properties form the foundation of material science, influencing how substances respond to external forces and temperature changes. In a world increasingly reliant on advanced technologies—from aerospace engineering to everyday consumer products—the ability to characterize and predict material behavior has become more important than ever [1-8].

The mechanical properties of materials, such as elasticity and strength, determine how they deform under stress and strain. Elasticity, the ability of a material to return to its original shape after deformation, is crucial in designing everything from bridges to electronic devices. Similarly, thermodynamic properties, such as thermal expansion and melting point, influence how materials perform under varying temperature conditions. These factors are critical in industries that demand materials capable of withstanding extreme environments, such as automotive, aerospace, and electronics manufacturing [9-18].

In recent years, the integration of computational methods, such as Density Functional Theory (DFT), has revolutionized the way researchers investigate these material properties. DFT allows scientists to model and simulate the atomic and molecular behavior of materials under different conditions, providing insights that are difficult or impossible to obtain through experimental methods alone. This approach has opened new doors for optimizing material design and performance, particularly in emerging fields like nanotechnology and advanced manufacturing [19-30].

This article explores the fundamental principles governing the mechanical and thermodynamic behavior of materials, including elasticity, crystallography, and thermodynamic properties, with a focus on their practical applications in technology. By understanding these principles, we can push the boundaries of material science and pave the way for future technological advancements.

## 2. METHODOLOGY

In this study, the mechanical and thermodynamic behavior of materials is investigated using a combination of computational simulations and theoretical frameworks. Density Functional Theory (DFT), through the Quantum ESPRESSO software package, is employed to calculate the electronic, mechanical, and thermodynamic properties of crystalline materials by solving the Schrödinger equation using a plane-wave basis set and pseudopotentials. The study also applies elasticity theory, utilizing Hooke's Law to analyze stress-strain relationships and determine elastic constants such as Young's modulus, bulk modulus, and shear modulus. Both second-order (SOECs) and third-order elastic constants (TOECs) are calculated to capture the materials' linear and non-linear elastic responses, while averaging methods like Voigt and Reuss are used for polycrystalline materials. Thermodynamic properties, including thermal expansion and specific

heat, are computed using DFT, along with phonon dispersion calculations to assess lattice vibrations and thermal stability. Additionally, X-ray diffraction (XRD) simulations and reciprocal lattice analysis provide detailed insights into the materials' crystallographic structure [31-35]. Finally, the computational results are validated by comparison with experimental data, ensuring accuracy and reliability in the characterization of materials' behavior under mechanical and thermal stresses.

## 3. RESULTS AND DISCUSSION

We firstly selected the input file for decomposing the stress- strain relation between the prescribe materials like the Aluminum (Al), silicon (Si), Germanium (Ge), Carbon (C), Gallium Arsenide (GaAs), Boron arsenide (Bas), Aluminum arsenide (AlAs) and Indium arsenide (InAs).

We establish Quantum ESPRESSO as open-source tool for investigating the structural parameter, elastic properties and the ground state electronics by implemented two approaches based on basic numerical differentiation of the ground energy and the functionals of stress-strain relation by selective codes for prescribed materials as presented on the tables below:

Table-1: Lattice Parameter a (Å), Bulk Modulus (GPa), Derivative of Bulk Modulus B'; of the prescribed elements/ compounds: Al, Si, Ge, diamond-C, GaAs, AlAs, and BAs.

| Elements/ Compounds | Lattice Parameter | | Bulk Modulus | | Derivative of Bulk Modulus | |
|---|---|---|---|---|---|---|
| | This Work | Previous Reported Value | This Work | Previous Reported Value | This Work | Previous Reported Value |
| Al | 3.98 | 3.97 | 83.8 | 83 | 3.85 | - |
| Ge | 5.57 | 5.66 | 53.4 | 59 | 5.88 | - |
| Si | 5.38 | 5.43 | 91.6 | 83 | 4.18 | - |
| Diamond-C | 3.57 | 3.50 | 53.8 | 442 | 10.24 | - |
| GaAs | 5.57 | 5.60 | 75 | 75.20 | 4.33 | 4.81 |
| AlAs | 5.60 | 5.63 | 71.9 | 75.1 | 6.33 | 4.51 |
| BAs | 6.32 | 4.74 | 101 | 147.5 | 3.52 | 4.21 |

Table-2: Elastic Stiffness Constants $C_{ij}$ ($GP_A$), Bulk Modulus B ($GP_A$), Shear Modulus G ($GP_A$), Young's Modulus E ($GP_A$) and Poisson Ratio $\vartheta$; of the prescribed elements/ compounds: Al, Si, Ge, diamond-C, GaAs, AlAs, and BAs.

| Elements/Compounds | Parameter | This Work | Previous Reported values |
|---|---|---|---|
| Al | $C_{11}$ | 111.77 | 107 |
| | $C_{12}$ | 69.81 | 61 |
| | $B$ | 83.8 | 83 |
| | $G$ | 21 | 25 |
| | $E$ | 58.14 | 70 |
| | $\vartheta$ | 0.38 | 0.31-0.34 |
| Ge | $C_{11}$ | 84.69 | 126 |
| | $C_{12}$ | 37.75 | 44 |
| | $B$ | 53.4 | 75 |
| | $G$ | 23.47 | 41 |
| | $E$ | 61.41 | 103 |
| | $\vartheta$ | 0.30 | 0.25 |
| Si | $C_{11}$ | 125.85 | 165.64 |
| | $C_{12}$ | 74.48 | 63.94 |
| | $B$ | 91.6 | 83 |

| | | | |
|---|---|---|---|
| | $G$ | 25.69 | 50.92-79.4 |
| | | 70.48 | 130.2-187.5 |
| | $\vartheta$ | 0.37 | 0.064 to 0.361 |
| Diamond-C | $C_{11}$ | 77.16 | 1079 |
| | $C_{12}$ | 42.12 | 124 |
| | $B$ | 53.8 | 442 |
| | $G$ | 17.52 | 478 |
| | $E$ | 47.41 | 1050 |
| | $\vartheta$ | 0.35 | 0.1 |
| BAs | $C_{11}$ | 172.68 | 295 |
| | $C_{12}$ | 65.16 | 78 |
| | $B$ | 101 | 152 |
| | $G$ | 53.76 | - |
| | $E$ | 137 | - |
| | $\vartheta$ | 0.26 | - |
| AlAs | $C_{11}$ | 110.7 | 116 |
| | $C_{12}$ | 52.50 | 55 |
| | $B$ | 71.9 | 75 |
| | $G$ | 29.10 | 31 |
| | $E$ | 76.92 | - |
| | $\vartheta$ | 0.32 | 0.324 |
| GaAs | $C_{11}$ | 122.11 | 138 |
| | $C_{12}$ | 51.44 | 55 |
| | $B$ | 75 | 75.5 |
| | $G$ | 35.33 | 28.9 |
| | $E$ | 91.60 | 63.0 |
| | $\vartheta$ | 0.30 | 0.36 |

Fitting the total energy for a cubic unit cell as function that depends on the volume of the unit cell were investigated by calculating the equilibrium structural parameter of the given materials for the equation of states.

Comparisons of the results with the previously available reported and experimental data with the data obtained from the investigation, were in good agreement

These results approve the suitability of chosen cell parameters and pseudopotentials in theoretical study of given crystalline materials.

These elastic constants are very important in strength, structural analysis of material. Also, they may help in finding velocity of longitudinal waves in medium and investigation of piezoelectric character.

In this work, we have focused on fcc and zinc blende structures. Later, other crystal structures (bcc, perovskite, wurtzite etc.) may also be studied, which were not included here due to paucity of space and time.

## 4. CONCLUSION

The theoretical framework of DFT methods has been found to be suitable for study of elastic constants. Theoretical studies help in preliminary investigation as well as verification of experimental data. The open-source software, Quantum ESPRESSO shows the usefulness for obtaining the elastic stiffness constants and determining the elastic moduli for solid-state materials, which in turn provides us the strength of the materials by understanding there structural behaviors in very less time spent. The selection of the input file and the relaxation of the geometry that converges for the selected material provides the proper information for the structural engineering of the given material. The calculated values from computational techniques are in fair agreement with the previously reported values for the prescribed elements/ compounds: Al, Si, Ge, diamond-C, GaAs, AlAs, InAs, and BAs.

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