Ab-initio study of structural and electronic properties of terbium

Abstract

In present work, the ground state and electronic properties of terbium (Tb) atom were revisited within the density functional theory. The local density approximation for exchange and correlation potential was used. The structure optimization has shown that terbium atom has a hexagonal type structure and obtained lattice parameters were comparable to the experimental and theoretical data. Furthermore, the electronic band structure and density of states were also obtained for the higher symmetry in the Brillouin zone and compared with available data.

Key Words: DFT, Band energy, Terbium, Fermi surface, Charge density.

Introduction

In the production of the electronic device, in a sonar system, sensor, in sound bud device, magneto- mechanical devices and even in colour T.V tubes Terbium metal is widely used [I-II]. Hence to understand their efficiency in devices the study of structural and electronic properties is essential [III]. Tb element basically has the hexagonal structure with space symmetry P63/mmc (194) [IV]. The noble work by K. M. Döbrich [V] has been carried out to study electronic band structure and Fermi Surface of Tb element. In which focus on the half- filled 4f shell take place. Therefore, a detail studies of structural properties of Tb is essential to improve theoretical understanding of electronic properties of the 4f metal. In the present work, structural properties and lattice parameter were computed also the computation of electronic band structure and Fermi surface takes place to understand its metallic and ferromagnetic characteristic at 0K. Further charge density also plotted to understand the distribution of electron between Tb metal. The rest of this paper is organised as follows: The introduction section, the computational method, the result of calculation and discussion and final conclusion of the work.

Computational method

Quantum espresso code is used to perform calculation based on density functional theory with plane-wave self- consistent field (PWSCF) method [VI-VII]. To take care of the exchange and correlation effects the local density approximation (LDA) [VIII]. The separation energy between core and valence state was define by cut-off energy, and taken as 200 Ry. The Tb ([Xe] 4f9 6s2) orbits was treated as valence state. Self-consistency for Terbium obtained using 10×10×10 K-point in the irreversible Brillouin zone, consider without spin polarization. We have taken a0 6.2125 au and c0 9.7455 au as the absolute lattice constant for the computation. The self-consistent calculation is considered to be converging when the computed energy changes by less than 10^{-3} Ry.

Result and Discussion

The acceptable unit cell for the terbium (Tb) with space symmetry P63/ mmc and space group is (194) [IV] is shown in Fig 1(a) and Fig 1(b) represents the first Brillouin zone (BZ) along high symmetric direction. The total energy verses lattice parameter (au) is fitted with the non-linear Murnaghan equations of states [IX]. The energy verses lattice parameter curve of Tb for LDA is shown in Fig 2. The computed equilibrium lattice parameter (a0), bulk modulus (B0), first order
pressure derivative ($B'_0$) and total energy ($E_0$) are also summarized in Table 1 with available experimental data. The computed parameters are in comparison with experimental results which proposed that the occurrence of over binding in the LDA. Hence, the lattice parameter and bulk modulus ($B_0$) using LDA approximation also observed in several similar systems in other simulation.

![Fig. 1. (a)](image-url) The compound crystal of Tb the large spheres represent rare earth atoms. (b) standard shapes of Brillouin zone for Tb with unit cell space group P63/mmc (194) plotted with Xcrysdan [X].

![Fig.2](image-url) Total energy of Tb atom as a function of lattice parameter $a_0$ and $c_0$.

**Table 1.** Equilibrium lattice constant $a_0$, bulk modulus $B_0$ (in GPa), pressure derivative $B'_0$ and total energy compared to experimental data.

<table>
<thead>
<tr>
<th>Tb</th>
<th>Lattice parameter (au)</th>
<th>$B_0$ (GPa)</th>
<th>$B'_0$ (GPa)</th>
<th>$V_0$ (au)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>6.2125</td>
<td>44.2</td>
<td>1.00</td>
<td>$59.944 \times 10^{-3}$</td>
</tr>
<tr>
<td>$c_0$</td>
<td>9.7455</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Experimental**

| $a_0$  | 6.878 [XI]    | 38.7 [XII] |
| $c_0$  | 10.703        |            |

It is essential to investigate the electronic band structure and density of states of material because these properties are closely associated to the most macroscopic properties of the material. The
calculated band structure at equilibrium lattice constant for a different high-symmetry direction in the Brillouin zone and the total density of state of Tb at 0K is shown in Fig. 3. The position of $E_F$ in the electronic band structure predicts the metallic nature of Tb as several bands cross the Fermi level ($E_F$). Electronic bands are dispersive in nature indicating high electron mobility which shows an additional characteristic of metallic behaviour. The DOS is essential to characterised the number of different states at a particular energy level that electron is allowed to occur. It is mathematically represented by density distribution and it is generally an average over space and time domain of the various states occupied by the system. The density of the state is important electronic properties as it shows electrons charge distribution for a given dimension. We also measure the density of state due to the vibrational frequency of some of the atom which is investigated in Partial Density of States. Fig – represent the sharp peaks below the Fermi level are mainly due to the hybridization of f- Tb states. In DOS, the significant peak on Fermi level in the region of the conduction band is mainly due to the involvement of f-Tb.

![Diagram](image)

**Fig3.** (a) - Electronic band structure along high symmetry directions of Tb atom, (b) Total Density of state of Tb atom and (c) Partial density of state.

Charge density describes how much electric charge is accumulated in a particular field. Specifically, it finds the charge density per unit volume. It measures the amount of electric charge per unit volume of space in one, two and three dimensions. The total charge density plot is computed in the diagonal plane of the structure using Xcrysden [X]. Different colour represents
the loss and gain of an electron between Tb atoms. It can be seen from fig. 4 attractive power around Tb atoms is very high compared to surrounding hence it represents ferromagnetic behaviour of Tb atom [XIII]. Hence terbium is used in a wide variety of devices essential to an everyday life e.g. electric motor, generator, transformer, telephones and loudspeakers. From fig 4 the presence of yellow colour interstitial region between Tb atoms and on corners is represent metallic bonding between Tb atoms. The interstitial region represented by red colour indicate week metallic region around the atoms.

**Fig 4.** Total charge density plot of Tb atom at 0k along X-Y-Z plane. Charge density is in arbitrary units. Colour code is display in the figure.

The Fermi surface is the surface in reciprocal space which separates occupied from unoccupied electron states at 0K. The existence of a fermi surface is a direct consequence of the Pauli exclusive principle, which allows a maximum of one electron per quantum states [XIV]. Hence to understand electronic properties, we have computed fermi surface of Tb atom within the framework of Density Functional Theory in Quantum ESPRESSO code. The Fermi surface are plotted using Xcrysden [X]. It is observed the topology from Fig. 5(a-e) indicate the Fermi surfaces of Tb. From the figure, it is evident that Tb has Fermi surface state crossing the E_F. Fig 5(b) topology of Fermi surface is open Fermi surfaces due to significant crossing along K-Γ direction. Such open structure indicates that the Fermi surface of Fig. 9 reaches the boundary of first Brillion zone.

**Conclusions**

The work introduce in this paper aimed to establishing a picture of the electronic structure of Tb. Calculations performed using the PAW-SCF method as implemented in the Quantum espresso code have led to the following conclusions. Computed ground structure properties of Tb which mainly include equilibrium lattice constant, bulk modulus and first order pressure derivative are in accordance with the available experimental results. As Tb is ferromagnetic, so perfect study for band structure and density of state take place. From the band structure as it crosses the Fermi level which indicate its metallic characteristic and from PDOS of Tb one of the major conclusions is that f-Tb electron is significantly contributing to the total density of state. The charge density plot
for Tb atom indicate attractive power around Tb atoms type, hence it represents ferromagnetic behaviour of Tb atom and Fermi energy which explain metallic property at different high symmetry point of the Brillouin zone.

**Acknowledgement**

Authors acknowledge Computer facility developed under DST-FIST Level-I programme of Department of Science and Technology, Government of India, New Delhi and support under DRS-SAP-I of University Grants Commission, New Delhi.

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