© 2018 IJSRSET | Volume 4 | Issue 1 | Print ISSN: 2395-1990 | Online ISSN : 2394-4099
Themed Section : Science and Technology

Study of Electronic, Acoustical and Elastic properties of CdCe

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ABSTRACT

Elastic, acoustical and electronic properties of CdCe have been performed using the full-potential augmented plane-waves + local orbital (FP-LAPW + lo) method. The equilibrium lattice parameter, bulk modulus and its pressure derivative have been obtained using optimization method within generalized gradient approximation (GGA). Young's modulus, shear modulus, Poisson ratio, acoustical velocities for longitudinal and shear waves, Debye average velocity, Debye temperature and Grüneisen parameter have also been calculated. From electronic calculations, it has been found that electronic conductivity in CdCe is mainly caused by d-orbitals electrons of Cd with small contribution of Ce p-orbitals.

Keywords : Elastic Properties, Electronic Structure of Metals and Alloys, Ab-Initio Calculations

I. INTRODUCTION

Cadmium cerium (CdCe) has cesium chloride structure with the space group O_h^1-Pm3m (No. 221).In CdCe unit cell the atoms occupy at the positions:

Cd: (0, 0, 0)
Ce: (1/2, 1/2, 1/2)

The calculated lattice constant and density of CdCe, a = 3.865 $\overset{o}{A}$ and d = 7.262 g/cm^3 as reported in reference [1].

Elastic properties of materials are directly related to their microstructure as they determine the response of the crystal to external forces, as characterized by bulk modulus, shear modulus, Young's modulus, and Poisson' s ratio, and obviously play an important role in determining the strength and stability of materials [2]. The elastic constants of materials are used to obtain the several other physical parameters viz. acoustic attenuation, Debye temperature, Debye average velocity, Grüneisen parameter, nonlinearity coupling constants, thermal relaxation time, phonon viscosity and other physical properties of materials. Therefore, these are of great interest in applications where the mechanical strength and durability are important [3].

The electronic structure provides information on the density of states (DOS) of the valence, conduction bands, charge density, and ionic charges as well as the prediction and description of the ground state properties of materials such as metals, semiconductors, and insulators [4]. Thus structural, elastic constants (viz. equilibrium lattice parameter, bulk modulus and its pressure derivative, Young's modulus, shear modulus, Poisson ratio), electronic calculations (viz. density of states, electronic charge) and some other related parameters like sound velocities for longitudinal and shear waves, Debye average velocity, Debye temperature and Grüneisen parameter of the cubic CdCe have been investigated by reliable ab initio method that is the base on density functional theory (DFT).

Computational detail

The full-potential linear augmented plane wave + Lo (FP-LAPW + Lo) method [5] has been used to calculate the total energies as well as the ground state properties. Generalized Gradient Approximation (PBE-GGA) based on Perdew-Burke-Ernzerhof (PBE) [6] has been used to determine the optimized structure of the compound CdCe. In this method, the basis set is obtained by dividing the unit cell into non-overlapping atomic spheres and an interstitial region. Inside the atomic sphere a linear combination of radial function times the spherical harmonics is used; in the interstitial region, a plane wave expansion is augmented by an atomic like function in each atomic sphere. The generalized gradient approximation parameterized by Perdew et al. [7] is used for calculating the exchange and correlation energy. The total energies are fitted to Murnaghan, equation of state [8] to obtain the ground state properties (lattice parameter, bulk modulus and its pressure derivative) and elastic constants, which in turn have been used to obtain the Youngs modulus, shear modulus, Poisson ratio, sound velocities for longitudinal and shear waves, Debye average velocity, Debye temperature and Grüneisen parameter.

In a cubic crystal, there are three independent elastic constants, namely, C_{11}, C_{12} and C_{44}. As a result, a set of three equations is needed to determine all the constants. Hence, three types of strain must be applied to the starting crystal [9, 10].

(i) The first type strain involves calculating the bulk modulus, given by the formula

$$B_0 = (C_{11} + 2C_{12})/3 \tag{1}$$

(ii) Second type strain involves performing volume conservative tetragonal strain given by the following tensor.

$$\begin{bmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \dfrac{1}{(1+\varepsilon)^2} - 1 \end{bmatrix} \tag{2}$$

This strain has an effect on the total energy from its unstrained state given by following equation.

$$E(\varepsilon) = E(0) + 3(C_{11} - C_{12})V_0\varepsilon^2 + o(\varepsilon^3) \tag{3}$$

(iii) Finally, for the third type of deformation, we use the volume conserving rhombohedral strain tensor given by

$$\frac{\varepsilon}{3}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \tag{4}$$

This volume conserving rhombohedral strain transforms the total energy to

$$E(\varepsilon) = E(0) + \frac{1}{6}(C_{11} + 2C_{12} + 4C_{12})V_0\varepsilon^2 + o(\varepsilon^3) \tag{5}$$

Once we have calculated three elastic constants namely C_{11}, C_{12} and C_{44}, bulk modulus, B (see equation(5)), Young' s modulus, Y, isotropic shear modulus, G and Poisson ratio, ν .(which are important fundamental parameter closely related to many physical properties viz. internal strain, thermoelastic stress, sound velocity, fracture toughness) can be calculated easily using the following explicit expressions [11]:

$$G = (G_V + G_R)/2 \tag{6}$$

Here G_V is Voigt' s shear modulus corresponding to the upper bound of G values, and G_R is Reuss' s shear modulus for cubic crystals corresponding to the lower bound values, expressed as:

$$G_V = (C_{11} - C_{12} + 2C_{44})/4 \quad (7)$$

$$G_R = 5[(C_{11} - C_{12})C_{44})]/[4C_{44} + 3(C_{11} - C_{12})] \quad (8)$$

$$Y = \frac{9GB}{G + 3B} \quad (9)$$

$$\nu = (3B - 2G)/(6B + 2G) \quad (10)$$

Sound velocity depends upon second order elastic constants and mass density. Therefore, sound velocity for longitudinal and shear waves (V_L and V_S) and Debye average velocity (V_m) can be obtained using calculated elastic moduli and mass density. The explicit expressions are as follows [12]:

$$V_L = \sqrt{\frac{3B + 4G}{3\rho}} \quad (11)$$

and

$$V_L = \sqrt{\frac{G}{\rho}} \quad (12)$$

$$V_m = \left[\frac{1}{3}\left(\frac{1}{V_L^3} + \frac{2}{V_S^3}\right)\right]^{-1} \quad (13)$$

The Debye temperature, θ_D and Grüneisen parameter, ς are two useful parameters in solid state problems because of their inherent relationship to lattice vibrations. The Debye temperature θ_D can be used in characterizing the excitation of phonons and to describe various lattice thermal phenomena and Grüneisen parameter describes the phonons contribution to specific heat.

Debye temperature, θ_D [12] and Grüneisen parameter, ς [13] are sound velocity and mass density dependent, which are calculated using the expressions given by

$$\theta_D = \left(\frac{\hbar}{k_B}\right)\left[\frac{3n}{4\pi}\left(\frac{N_a\rho}{M}\right)\right]^{1/3} V_m \quad (14)$$

$$\varsigma = \frac{9(V_L^2 - \frac{4}{3}V_S^2)}{2(V_L^2 + 2V_S^2)} \quad (15)$$

Here $(\hbar = h/2\pi)$ h being the Plank Constant and κ_B is Boltzmann constant.

To obtain the structural ground state parameters viz. equilibrium lattice constant, bulk modulus and its pressure derivative, total energy has been fitted to the Murnaghan equation of state [8] and the total energy has been plotted as a function of reduced volume for CdCe. The plot connecting the total energies to relative volumes for the compound is shown in Figure 1. The calculated ground state properties viz. equilibrium lattice constant, bulk modulus and its pressure derivative are tabulated in Table 1.

Table 1 Calculated lattice constant, a_0 ($\mathring{A}$), bulk modulus, B_0 (GPa), its pressure derivative, B_0', elastic moduli for CdCe using GGA functional.

	a_0	B_0	B_0'
Present	3.79	44.18	5.17
Ref. [1]	3.85	------	-----

No experimental values of the equilibrium bulk modulus (B_0) and its pressure derivative (B_0) are available in literature, thus, no comparison can be made for B_0 and B_0 for CdCe. However, value of lattice constant (a_0) is available in the literature [1] which is in good agreement with calculated value of lattice constant (Table 1). Present calculations are based on the density functional theory within the framework of the GGA, which is sufficiently accurate in predicting the ground state properties.

Table 2. Calculated elastic moduli, C_{ij} (GPa), Bulk modulus, B (GPa), Young's modulus, Y (GPa), otropic shear modulus, G (GPa), Poisson ratio, v for CdCe using GGA functional.

C_{11}	C_{12}	C_{44}	B	Y	G	ν	B/G
56.51	18.02	16.94	44.18	36.22	13.09	0.36	0.29

Table 3. Calculated, Mass density, ρ (gm/cm^3), sound velocities (10^3 m/sec) for longitudinal and shear wave (V_L and V_S), Debye average velocity, V_m (10^3 m/sec), Debye temperature, θ_D (K) and Grüneisen parameter

ρ	V_L	V_S	V_m	θ_D	ζ
7.32	2.90	1.34	1.51	242	2.24
7.22 [1]	----	----	----	----	----

The calculated elastic moduli are given in Table 2. The elastic stability criteria for a cubic crystal [4] at ambient conditions can validate our calculations for elastic moduli. At ambient conditions the stability conditions are C_{11}-$C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$ including the cubic condition $C_{12} < C_{11}$ and $C_{12} < B < C_{11}$. Since, our calculated values of C_{11}, C_{12} and C_{44} satisfy the elastic stability criteria, Therefore, justifying the calculated values of elastic moduli.

Bulk modulus, B isotropic shear modulus, G Young' s modulus, Y and Poisson ratio, ν are also the important physical parameters, which tell more about the mechanical stability, hardness, brittle and ductile properties of materials. The calculated values of B, G, Y and ν are given in Table 2. For covalent and ionic materials, the typical relations between bulk and shear moduli are G = 1.1B and G = 0.6B [10], respectively. In our case, the obtained factor relating the bulk and shear moduli is less than the condition G=0.6B and approaching to ionic condition, found to be 0.29, indicating weaker ionic bonding in CdCe. Poisson ratio gives the ductile or brittle behavior of material. The compounds for which ν > 0.30 are brittle otherwise ductile [10]. Poisson ratio for CdCe is 0.36, reflecting brittle character.

The mass density (ρ), sound velocities for longitudinal and shear waves (V_L and V_S), Debye average velocity (V_m), Debye temperature (θ_D) and acoustic Grüneisen parameter (ζ) of a crystal are also the material parameters associated with lattice vibrations, which are basically depend upon the elastic moduli. In the present work, the calculated values of ρ, V_L, V_S, V_m, θ_D and ζ have been presented in Table 3. Only the value of mass density is available in literature [1], which is in good agreement with our calculated value of mass density. Since the values of V_L, V_S, V_m, θ_D and ζ have been calculated from the elastic constants using the first principle theory (which is most reliable theory), therefore, we beleive that our calculated values of V_L, V_S, V_m, θ_D and ζ are valid.

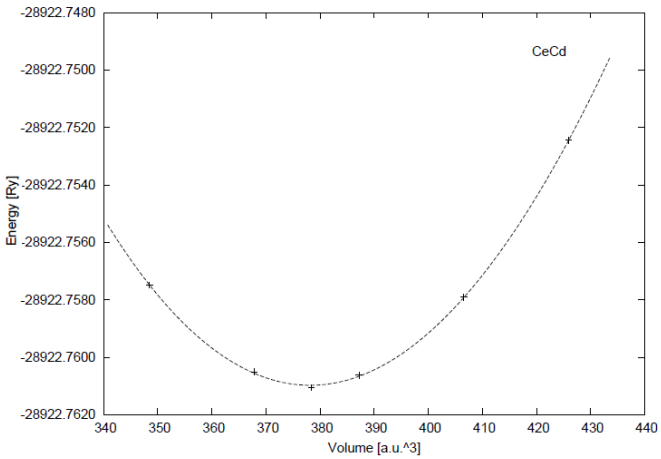

Figure 1. Total energy as a function of volume for CdCe with GGA calculation

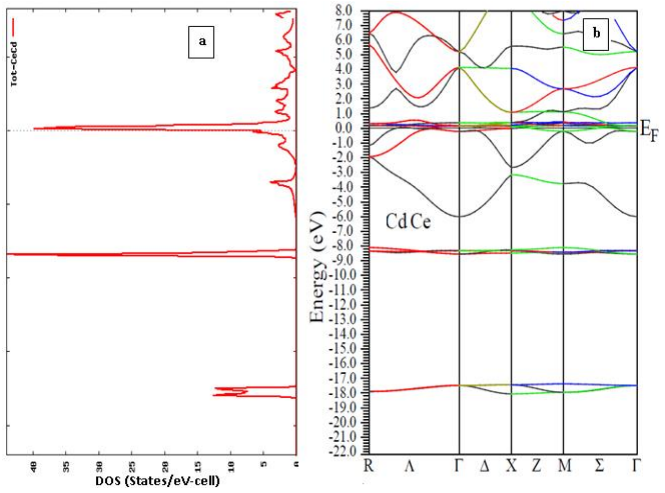

Figure 2 (a) calculated total density of states and (b) self-consistent electron dispersion curve along symmetry direction in the Brilloun zone for CdCe with GGA calculation.

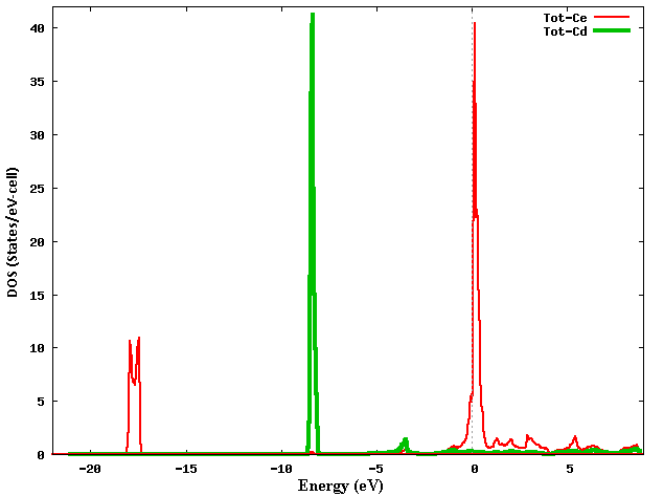

Figure 3. Calculated total density of states for Ce and Cd

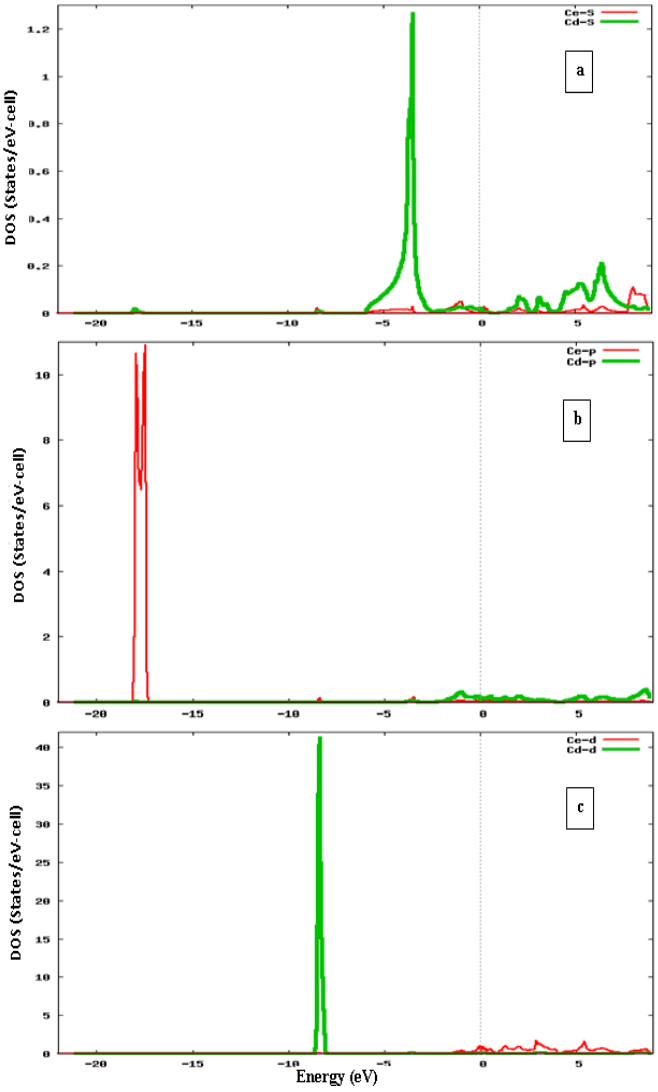

Figure 4. Calculated partial density of states for Ce and Cd for (a) s-states (b) p-states (c) d-states

Figure 2 consists (a) calculated total density of states and (b) self-consistent electron dispersion curve along symmetry direction in the Brilloun zone for CdCe. It is clear from Figure 2 that there are total three bands at around -18 eV, -8.2 eV and -4 eV below the Fermi level.

Figure 3 shows the calculated total density of states for Ce and Cd atoms which indicates that Cd dominants over the Ce in contribution to electrical conductivity. Figure 4 shows the calculated partial density of states (for s, p, d states) for Ce and Cd respectively. It is clear from Figure 4 that lowest-lying band (at around -18 eV) arises from the Ce p-states and the bands lying above this (at around -8.2 eV) is mainly contributed by the d-like states of the Cd atom. Well above these, the bands (at around -4 eV) arise from the Cds states

Therefore, Cd d-states play key role in contribution to electrical conductivity with small contribution of Ce p-states (Figure 2-4).

II. CONCLUSION

The ground state properties have been calculated from ab initio method. The Young's modulus, shear modulus, Poisson's ratio, Debye temperature, sound velocity, Grüneisen parameter and other elastic properties were also calculated for CdCe compound for the first time. Calculations presented in this study also provide reliable description of total charge densities and partial densities of states for CdCe. D-states of Cd in CdCe are dominant over Ce p-states (Figure 4) in contribution to electrical conductivity in this compound. However, No experimental / theoretical data is available in literature related to the studied properties in the present paper on this compound. Present results may provide the guide for future experimental / theoretical calculations for experimentalists and theoreticians working in this field.

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