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Structural, Elastic, and Electronic Properties of Holmium based Compounds HoX_3 (X = Pd, Pt)

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The elastic, electronic, and structural features of the binary intermetallic compounds HoX_3 (X = Pd, Pt) are theoretically studied using density functional theory. The implications of include the exchange-correlation potential is investigated using a generalized gradient approximation with an extra Hubbard-U component to account for the Coulomb on-site interaction (GGA+U). Elastic constants of these compounds are calculated, and their anisotropic properties are examined. In addition, additional essential factors such as the Poisson's ratio, Young moduli, Shear moduli, Bulk moduli, and Cauchy pressure are studied. These compounds are both ductile and mechanically stable. Their band structures and state occupancy in spin-up and spin-down modes show the metallic character of these compounds.

Keywords: Intermetallic compounds, Electronic properties, Structural Properties, Elastic properties

INTRODUCTION

Intermetallics are distinctive materials consisting of two (or more) kinds of metal (or metal and nonmetal) atoms that exist as solid compounds and vary structurally from the essential components. Intermetallic-based alloys have many distinct characteristics when compared to ordinary metals and alloys. Traditional materials are made up of metallic or nonmetallic components solidified in a metal lattice. Atoms in typical alloys are held together by relatively weak metallic connections. Strong ionic and covalent bonding occurs in a crystalline lattice in the case of organized intermetallic. Furthermore, atoms always assume their specific places in a crystalline lattice, creating a so-called ordered superlattice with a long-range order (LRO) that is stable up to a critical ordering temperature.[1−5] These structural features are responsible for intermetallic's physical and mechanical qualities, including a very high melting point, a high strength (particularly at higher temperatures), and a relatively low elasticity. Because of these characteristics, they are comparable to ceramics. However, unlike ceramic materials, intermetallics have a metallic sheen, excellent thermal and electric conductivity, and some sensitivity to plastic deformation, indicating that they are metallic materials.[1,6,7]

Those compounds have helped to improve several fields of science and engineering. Because of their high internal order and mixed (metallic and ionic/covalent) binding nature, these compounds show appealing superconducting, chemical, and magnetic properties. They have a wide range of uses because of these properties, including superconductors (due to their excellent conductive nature), permanent magnets (because of their ferromagnetic activity), and furnace hardware (because of high melting points and thermal stability)[8]. To produce the strongest artificially induced magnetic fields, holmium alloys are utilized as magnetic flux concentrators. It is also used for nuclear control rods in nuclear reactors. As a yellow gas colorant, holmium oxide is employed. Holmium has no biological function and is one of the least prevalent elements in the human body. Even though it seems to have a low acute toxic value, holmium has been shown to promote metabolism.[1] To investigate the acoustic, electrical, elastic, and structural characteristics of $ScPd_3$, $ScPt_3$, and $ScRh_3$ compounds. These compounds exhibit metallic properties, according to their observations. According to Arıkan N et al.,[7,9] cubic inter-metallic compounds such as $LaPd_3$ and YPd_3 are more appropriate than other compounds because of their conducting, structural, and electrical characteristics as their mechanical reaction to external forces. YPd_3 magnetic, structural, and transport properties were investigated by Chen et al.[10] These molecules have also become crucial in hydrogen storage applications.[11] In a strong magnetic field, these materials usually show diamagnetic behavior. Many intermetallic compounds have an appealing mix of physical and mechanical characteristics, such as a high melting point, low density, and resistance to oxidation or corrosion. They have many uses in the aerospace sector, aviation engines, biomedical instruments, microelectronics, electronics, batteries, hydrogen storage systems, and chemical industries. A layer comprising one or more intermetallic compounds is present in every solder junction between the solder and the system of interest.[7–9]

Over the past several decades, significant effort has been made to increase the critical temperature Tc of superconductor materials. Compounds having an A-15 type structure are widely known to produce superconductivity, and the physical characteristics of these compounds affect the superconducting parameters. The A-15 family of A3B compounds has been widely investigated theoretically and empirically in this context[11–15], and thorough reviews of its intriguing characteristics have been published. The current research concentrated on the intermetallic compounds HoX_3 (X= Pd, Pt) based on Holmium. The elastic, structural, and electronic characteristics of HoX_3 (X= Pd, Pt) are calculated using the DFT framework's full potential linearized augmented plane wave (FP-LAPW). This research will aid in understanding the characteristics of the substances as mentioned above. It will close a theoretical research gap in these molecules' structure and elastic properties.[16–18]

COMPUTATIONAL DETAILS

HoX_3 (X= Pt, Pd) crystallizes in an $AuCu_3$-type cubic structure with the space group Fm-3m (225). The atoms in its unit cell are arranged in Wyckoff position order, with atom Ho occupying the cube's corners at (0,0,0) and X = Pd or P is occupying each face of the cube at (0.5, 0, 0.5), (0, 0.5, 0.5), and (0, 0.5, 0.5). (0.5, 0.5, 0). Figure 1 depicts the unit cell structure of this chemical. Another research used density functional theory in its framework. The FP-LAPW technique, as implemented in the WIEN2K code[19,20], is used for the calculation. The total energy was calculated using the generalized gradient approximation (GGA) with the inclusion of the Hubbard-U component to account for the on-site Columbic interaction modeled by Perdew, Burke, and Ernzerhof.[21,22] The structural optimization and the investigation of the structural parameters are carried out by fitting the technique of energy versus volume through Burch Murnaghan's equation.[23]

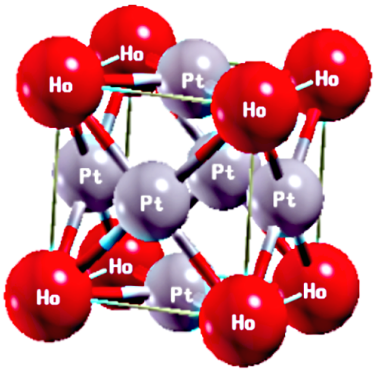

Figure 1. Unit cell structure of HoX_3.

The Kohn–Sham equations are self consistently solved to calculate the density of states for both spin-up (↑) and spin-down (↓) configurations. The energy difference between the core state and valence state is assumed as-6 Ry (Rydberg). The spherical harmonics with cutoff l-max = 10 inside the muffin-tin-approximation are used. Furthermore, the RMT value is chosen to be 2.5, K Point is selected to be 1000, and G-max is chosen as 12.

RESULTS AND DISCUSSION

This section explains the various characteristic properties of HoX_3 (X= Pd, Pt) intermetallic compounds.

Structural and Elastic properties

The HoX_3 (X= Pd, Pt) intermetallic compounds studied in this study exhibit a cubic crystal shape, as seen in Figure 1. Murnghan's equation[23] is used to study the ground state lattice characteristics, particularly the lattice constants. Figure 2 depicts the total energy variation as a function of volume. In

the instance of $HoPd_3$, the predicted lattice constant (4.10 Å) corresponds with the observed value[6]. Due to the absence of experimentally observed $HoPt_3$ equilibrium lattice constant values, we based our calculated values on the previously known $ScPt_3$ lattice constant.[7] Table1 lists the calculated values of the lattice parameters.

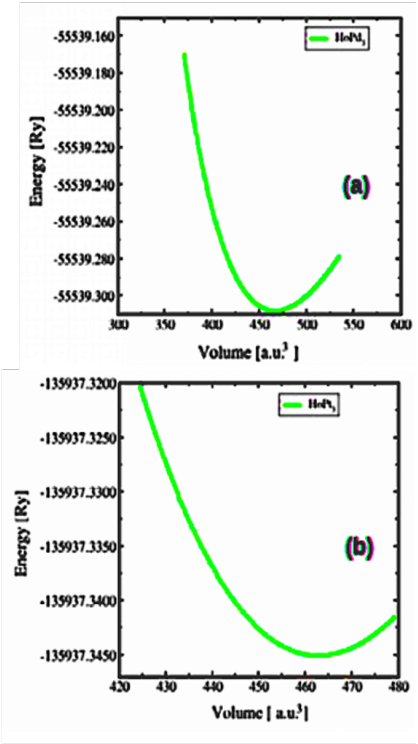

Figure 2. Total energy dependence of (a) $HoPd_3$ (a) $HoPt_3$ compounds

Elastic constants show the crystal's reaction to an external force and may provide important information about the mechanical characteristics of the solid material. Elastic constants govern the structure's stability, anisotropic properties, and crystal binding. Because the studied compounds have cubic crystal structures, we only require the three elastic constants values (C_{11}, C_{12}, and C_{44}) in the C_{ij} tensor to explain the elastic nature of these compounds. The C_{11} value for $HoPd_3$ is higher than the C_{11} value for $HoPt_3$, indicating that $HoPd_3$ is more elastic than $HoPt_3$. $HoPd_3$ also has a more significant transversal expansion (C_{12}) and stiffness (C_{44}). All three elastic constants are calculated and have positive values, as shown in Table I.

These compounds satisfy the Born-Haung (BH) stability criterion[24], as shown in the following equation. The table shows that all the calculated elastic constants values are positive, indicating that they meet the requirements.

$\mathbf{C_{11}, C_{44} > 0, C_{12} < B < C_{11}}$

$\mathbf{(C_{11}- C_{12}) > 0, (C_{11} + 2C_{12}) > 0}$

Other elastic parameter values, such as Bulk Modulus (B), an-isotropy factor (A), Young's modulus E, Poisson ratio (v), and Pugh index ratio (B/G), are calculated using the mathematical formulas shown below.[25] Table 1 displays the calculated values of these parameters.

$$B = \frac{C_{11} + 2C_{12}}{3}$$

$$A = \frac{2C_{44}}{C_{11} - C_{12}}$$

$$E = \frac{9BG}{3B + G}$$

$$\nu = \frac{3B - 2G}{2(2B + G)}$$

$$G = \frac{G_v + G_R}{2}$$

$$G_v = \frac{C_{11} - C_{12} + 3C_{44}}{5}$$

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}$$

The compounds are categorized as ductile or brittle based on the Poisson (v) and Pugh index (B/G) ratios[26,27]. The values of B/G and for HoX_3 (X= Pd, Pt) in this study are higher than their threshold values, which are 1.75 for B/G and 0.26 for Poisson ratio, indicating ductile behavior.

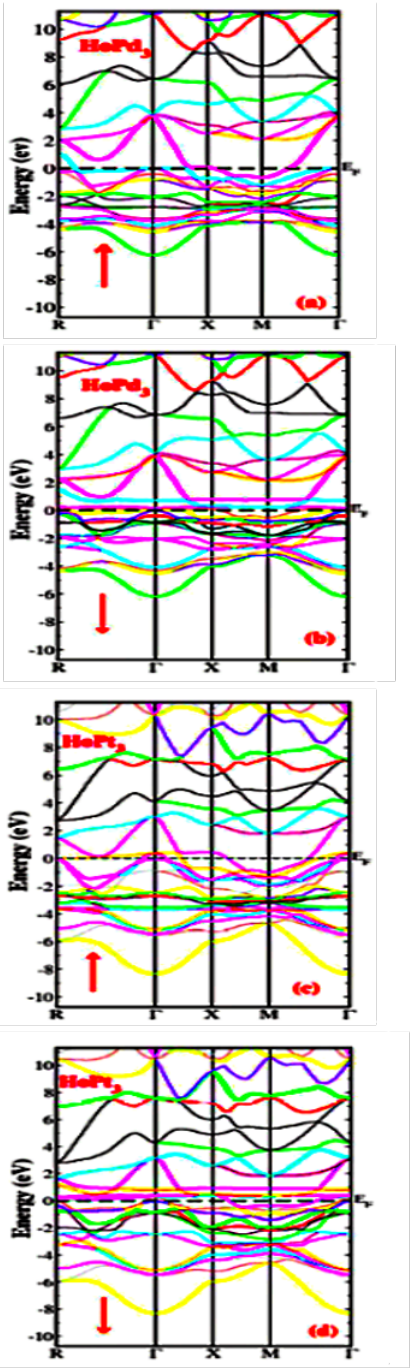

Figure 3. (a-d) The band structures of AB_3 intermetallic compounds (A = Ho and B = Pd, Pt) for both spin-up and spin-down channels.

Electronic properties

Figure 3 shows the spin-polarized band structures of HoX_3 (X= Pd, Pt) along high symmetry direction in the major-

Table 1. The computed values of lattice constants a_o (Å), elastic constants C_{ij} (GPa), an-isotropy factor [A, Bulk (B), Shear (G), and Young's (E)] moduli (all these moduli measured in GPa), Poisson ratio (ν) and Pugh ratio (B/G) at the equilibrium volume.

Compound	ao (A^o)	C11 (A^o)	C12 (A^o)	C44 (A^o)	AGPa)	GPa)	GGPa)	EGPa)	ν	B/G
HoPd3	4.1039	109.72	64.98	80.013	3.57	79.89	48.17	120.34	0.34	1.65
HoPt3	4.0958	170.32	61.71	76.13	1.40	97.91	66.49	162.65	0.30	1.47

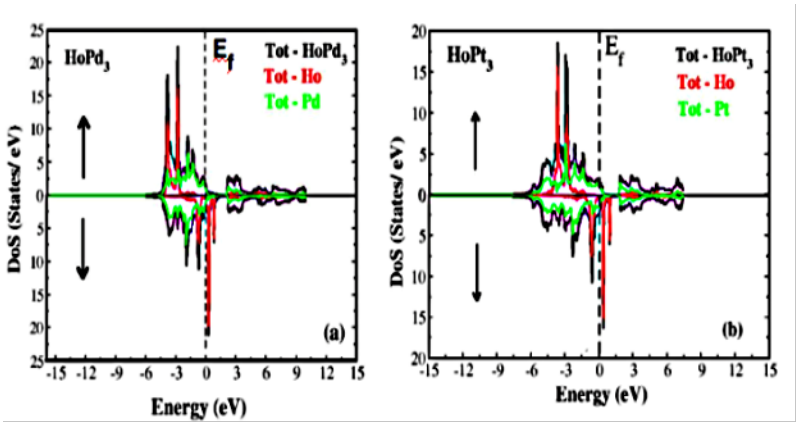

Figure 4. Density of states of HoX_3 (X=Pd, Pt).

ity (↑) and minority (↓) spins calculated using GGA+U. Overall, the band characteristics for each of these drugs are almost similar. These band profiles demonstrate that the conduction and valence bands significantly overlap in the majority and minority spins. No bandgap occurs at the Fermi level for these compounds, confirming their metallic character.[28,29]

The density of states (DOS) plots provide detailed information about the elemental contributions to the electrical structure of the studied molecule. Figure 4 depicts the total and partial density of states (TDOS, PDOS) of HoX_3 (X = Pd, Pt). According to this figure, the spin-up configuration states of Holmium (Ho) contribute significantly to the TDOS of both $HoPd_3$ and $HoPt_3$ in the valence band. In contrast, the conduction band is mainly occupied by states of Pd and Pt in the case of $HoPd_3$ and $HoPt_3$, respectively. However, in the spin-down state, Ho dominates both the conduction band and the valence area for $HoPd_3$ and $HoPt_3$.[30] The states of Pd and Pt in $HoPd_3$ and $HoPt_3$ are responsible for the metallicity of the respective compounds in both spin-up and spin-down configurations because they overlap at the Fermi energy level.

CONCLUSIONS

Using the GGA+U approximation, the DFT research was conducted to calculate the elastic, electronic, structural, and magnetic characteristics of HoX_3 (X = Pd, Pt) intermetallic compounds. The calculated lattice constant values match the experimental and theoretical data. Elastic parameters such as elastic constants, Bulk modulus, anisotropy factor, Poisson and Pugh ratios are also calculated. The Poisson ratio demonstrates the flexibility of the compounds under consideration. The calculated B/G ratio also supports flexibility. According to the band structure analysis and densities of states (DOS), these materials are metallic.

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