**Physical Characteristics of Metallic DyAg in B2 structure: A First-Principles Investigation**

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| **Abstract**The structural, elastic, electronic and thermodynamic properties of DyAg were investigated using the first-principles calculations. Presented herein are the outcomes pertaining to fundamental physical parameters, encompassing the lattice constant, bulk modulus, pressure derivative of bulk modulus, Zener anisotropy factor, Poisson’s ratio, Young’s modulus, and isotropic shear modulus by using generalized density approximation (GGA) method. The thermodynamic properties of DyAg were determined using the quasi-harmonic Debye model a range of 0-60 GPa and temperatures spanning 0-1000 K. The obtained results align with both experimental and theoretical values. |
| Keywords: Pressure effects, DyAg, Cubic, Thermodynamic properties, Elastic constants. |

1. **Introduction**

The rare earth elements (REE), including yttrium, fourteen lanthanide elements, and occasionally scandium, exhibit unique physical and chemical properties that make them indispensable in various critical technologies [1]. Rare earth elements are very important for many important technological developments such as catalysts, phosphors, glass and ceramics, lasers, and nuclear reactors. [2,3]

In recent years, numerous first-principles investigations have been undertaken to explore the structural, acoustical, elastic, electronic, and mechanical properties of rare-earth compounds [5-9], as well as specific intermetallics of note [9-10].

Given their industrial and technological importance, there remains a drive to explore novel intermetallic compounds that yield effective outcomes. In this ongoing investigation, a deliberate effort is being made to initiate a comprehensive examination of the structural, electronic, elastic, mechanical, and optical properties of relatively underexplored intermetallic compounds within the rare-earth-based DyAg system. The focus is on establishing correlations between the calculated properties of various substituents (Pd, Ag, and Cd) from the same

Despite the existence of theoretical research on DyAg compounds, there is a notable absence of data pertaining to the structural, elastic, and electronic properties of DyAg under pressure.

1. **Method and Calculations**

Theoretical computations were conducted utilizing the Vienna Ab initio Simulation Package (VASP) [11]. The study relies on Density Functional Theory (DFT), a quantum mechanics-based approach commonly applied in materials science and condensed matter physics. To enhance accuracy, gradient-corrected functionals were implemented, specifically adopting the Generalized-Gradient Approximation (GGA) proposed by Perdew and Wang [12]. Interaction modeling between ions and electrons employed the projector-augmented wave (PAW) method developed by Blöchl. Employing a plane-wave basis with an energy cutoff set at 900 eV ensured a robust foundation for the calculations. The Monkhorst and Pack [13] grid facilitated the sampling of the Brillouin zone, generating k-points distributed in an 18x18x18 pattern. Estimation of elastic constants was achieved through the application of the stress-strain method [14]. Vibrational properties were scrutinized by calculating phonon frequencies using the PHONOPY code [15, 16]. Phonon frequency calculations were enhanced through the utilization of the supercells approach, allowing for a detailed analysis in more complex structural scenarios.

1. **Results and Discussion**
	1. **Structural and mechanical properties**

The intermetallic compound DyAg adopts the CsCl crystal structure, characterized by a space group of 221 (pm3m). This structural arrangement comprises two interlocking sublattices housing anions and cations. In this system, one ion is positioned at the center of the cube, while the other is surrounded by eight ions. The specific locations of Dy and Ag atoms in the unit cell are denoted as Wyckoff 1a(0,0,0) and 1b(0.5, 0.5, 0.5), respectively (see Fig.1). Upon the creation of an atomic structure, geometric optimization was performed, revealing a determined lattice constant of 3.608 Å (refer to Table 1). Notably, this computed value aligns with theoretical predictions available in the literature. Table I provides insights into the bulk modulus, pressure derivative of the bulk modulus, and total energy values derived from energy-volume curves (Fig.1-b). To investigate the impact of pressure on DyAg, optimization runs were conducted within the pressure range of 0 to 60 GPa at 10 GPa intervals. The outcomes indicate a reduction in both lattice constant and volume with increasing pressure. Essentially, heightened pressure induces a contraction in the bond length between atoms, amplifying atomic interactions and resulting in a corresponding decrease in volume, as depicted in Fig. 1-c.

**Table 1.** Calculated lattice parameters, bulk modulus (B), pressure derivatives of bulk modulus (B’) formation for DyAg compound.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 0 GPa | a (Å) | B (GPa) | B` | Etot (eV/atom) |
| This studyTheory [8]  | 3.6083.608 | 66.74 | 4.44 | -4.0484 |

  

 (a) (b) (c)

**Figure 1.** (a) The unit cell of DyAg (b) The relationship between volume and total energy for DyAg (c) Changes in lattice parameter and cell volume of DyAg under varying pressure.

Elastic properties serve as crucial indicators, offering valuable insights into the bonding characteristics, flexibility, hardness, and mechanical stability of materials. In this study, we employed the stress-strain method to compute the second-order elastic constants for the cubic DyAg compound with a B2 structure. Table 2 presents the mechanical properties derived from these elastic constants. To investigate the impact of pressure, a range of pressures from 0 to 60 GPa was applied to the DyAg compound. The mechanical stability of the cubic system is determined by elastic constants C11, C12, and C44. Elastic stability, as per the Born criteria, is consistently met across all pressure values, ensuring the DyAg compound remains elastically stable.Notably, the DyAg compound exhibits resilience to unidirectional compression, particularly reflected in the elevated C11 value under varying pressures. The trend in Young's modulus (E) indicates an increase with pressure, highlighting the strengthening of covalent bonds and structural rigidity. In terms of ductility, the DyAg compound fulfills criteria such as B/G exceeding 1.75 and a Poisson's ratio (v) above 0.26, confirming its elastically ductile nature. Hardness, as measured by Hv, demonstrates an increasing trend with pressure, signifying heightened hardness levels in the DyAg compound under varying pressure conditions.

**Table 2.** Elastic constants (in GPa), isotropic shear modulus G, Young modulus E, G/B, Poisson ratio υ, and hardness Hν at different pressures in GGA approximation for DyAg under different pressures (GPa) at zero temperature.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **P** | **C11 (GPa)** | **C12 (GPa)** | **C44 (GPa)** | **G** | **E** | **G/B** | **ν** | **Hv****(GPa)** |
| 0 | 95.2 | 52.7 | 35.8 | 29.0 | 76.0 | 0.434 | 0.310 | 3.2 |
| 10 | 123.7  | 83.9  | 51.2  | 35.0  | 93.7  | 0.360  | 0.3391  | 3.8  |
| 20 | 146.0 | 113.8 | 63.9 | 36.9 | 100.7 | 0.296 | 0.365 | 4.1 |
| 30 | 165.3 | 142.6 | 75.0 | 37.3 | 107.9 | 0.241 | 0.388 | 4.5 |
| 40 | 183.1 | 170.1 | 85.7 | 39.2 | 116.3 | 0.196 | 0.407 | 4.8 |
| 50 | 200.0 | 196.3 | 96.0 | 40.3 | 121.7 | 0.158 | 0.420 | 5.4 |
| 60 | 217.3 | 221.9 | 106.1 | 48.4 | 138.3 | 0.128 | 0.438 | 6.1 |



**Figure 2.** Effect of pressure change on elastic properties of Cij(GPa).

* 1. **Electronic properties**

The evaluation of the electronic band structure serves to elucidate the physical, optical, and transport characteristics inherent in crystalline solids. Figure 3 illustrates the electronic energy band structure of DyAg along the high symmetry orientation GXMRX within the Brillouin region. The Fermi energy level was established at 0 eV for reference. Notably, the valence band maxima and conduction band minima overlap without any discernible gap, indicating the metallic nature of DyAg.

In Figure 4, the Density of States (DOS) values are presented. A noteworthy observation is the decrease in DOS intensity influenced by pressure. The pressure-induced narrowing of bond lengths between atoms leads to increased bond interactions. A non-zero DOS value confirms the metallic nature of the material.

This analysis of the electronic band structure and DOS provides valuable insights into DyAg's metallic behavior, shedding light on its response to external pressure and the resulting impact on bond lengths and interactions between atoms.

1.  b) 

**Figure 3.** The electronic band strıcture of DyAg.a) 0 GPa b) 60 GPa.

PDOS and TDOS data were plotted in Fig. 4 to analyze the contributions from the atoms to the bands. It can be divided into three parts, namely the valence band, the Fermi level, and the conductivity band. The greatest contribution to the valence band is Ag-d states, while it is from Dy-d at the Fermi level. In the conductivity band, Dy-d and Dy-p are more dominant. In addition, PDOS and TDOS peak intensities decrease with increasing pressure.

a) **** b) ****

**Figure 4.** Total density and partial density of states a) 0 GPa b) 60 GPa.

* 1. **Vibrational properties**

The phonon distribution of a compound provides insights into various critical physical properties of solid structures, including phase transitions, heat conduction, stability, and specific heat. Figure 5 illustrates the phonon distribution and phonon frequencies of the DyAg compound along the high-symmetry orientation of the first Brillouin zone at 0 GPa. In the DyAg compound, there are 6 modes, with 3 being acoustic and 3 being optical. Notably, the absence of negative modes in the phonon distribution curves signifies the compound's stability. There is no observed phase change in the compound as pressure increases, emphasizing its overall stability. Given the relatively low mass difference between Dy and Ag atoms, there is no discernible band gap between the acoustic and optical modes. Lattice vibrations play a pivotal role in energy absorption in solids, and the presented Partial Density of States (PDOS) graph on the right further elucidates this. Within the range of 0-2.5 THz, the heftier Ag atoms contribute significantly to the total PDOS in the acoustic background, while in the range of 2.5-4 THz, Dy makes the greatest contribution to the optical phonon. The observed flats in the phonon vibrations correspond to peaks in the Density of States (DOS), providing a comprehensive picture of the compound's vibrational and energy absorption characteristics.



**Figure 5.** The phonon dispersion curves and partial phonon density of states (PDOS) for the DyAg compound.

1. **Conclusion**

Employing the DFT method, we delved into the impact of pressure on the structural, elastic, electronic, and vibrational characteristics of DyAg. Initially exhibiting ductile and soft properties at ambient pressure, the alloy progressively hardened as pressure increased. With elevated pressure, DyAg exhibited a transition to metallic behavior. Notably, analysis of phonon data affirmed the dynamic stability of the compound. Our results underscore the mechanical and dynamic stability of DyAg under pressure, up to 60 GPa. In essence, this theoretical exploration scrutinizes the diverse effects of pressure on the myriad physical properties of DyAg within the B2 structure. We anticipate that our study will serve as a catalyst, inspiring researchers to conduct more comprehensive investigations into DyAg, encompassing both theoretical and experimental dimensions.

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