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Research Article

Computational Study for Band Structure Calculation of InPd Intermetallic

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Abstract. This paper reported the electronic and structural calculations of InPd at computational level. For studying these properties we have used Quantum Espresso code. The CsCl (B2-type) structure is where the current intermetallic crystallises. Calculations are made for the ground state parameters, including the lattice constant (a_0), bulk modulus (B), and its pressure derivative (B'). These findings are in good agreement with those that are currently available. In order to determine thermodynamical quantities, we have also examined Murnaghan's equation of state. Their ductility is confirmed by the current intermetallics.

Keywords. Intermetallics, Crystal structure, Electronic properties, Band structure, computational study

Mathematics Subject Classification (2020). 06B05, 74E15

1. Introduction

Materials that are light in weight, ductile, stiff, non-corrosive, and strong at high temperatures are required for current scientific applications. For experimentalists to be useful for high-tech application, computational science provides invaluable formative elements. Groups of lanthanides enable anything from electric vehicles and energy-efficient light bulbs to massive wind turbines and the potential for magnetic refrigeration in the future. The effect of intermetallic compounds on the mechanical and electrical properties of friction stir-welded Al and Cu busbar for battery pack applications is also investigated. Intermetallic compounds

have a wide reservoir of possible energy-related uses arising from optical, magnetic, caloric, electric, and catalytic capabilities. Understanding of chemical concepts can be improved by the discovery of new intermetallic compounds. In addition to producing innovative applications, these principles oversee structural stability and chemical bonding. A brittle intermetallic precursor combined with a particulate reactant metal is utilised to create an intermetallic-bonded ceramic composite principles of chemistry. The ordered intermetallic compounds, which are light in weight are technologically of use in high temperature properties such as creep resistance. To understand these properties the acquaintance of constitutional and thermal defects is requisite. for possible use as coatings or structural wear compounds on engineering steels. There has been discussion of intermetallic compounds (Ahmad *et al*. [1]).

Intermetallic compounds consistently offer unique properties that are superior to those of more traditional solid solution alloys with the same composition. For sophisticated and high-performance engineering applications, better understanding of the bonding in intermetallic compounds would greatly accelerate their growth. Physical properties of the InPd intermetallic catalyst have been reported by Wencka *et al*. [10]. Magagnosc *et al*. [6] reported using sputter deposition at high temperatures to achieve isocheimal control over mechanical characteristics and structural state in Pd-based metallic glass. A theoretical study of the surface structures of In-Pd intermetallic complexes was published by Gaudry *et al*. [2]. McGuirk *et al*. [7] detailed the atomic structure of the low-index surfaces of the intermetallic complex InPd. To guide the catalytic characteristics of intermetallic compounds and alloys in reforming reactions, a controlled in situ breakdown and self-activation study was carried out (Penner and Nezhad [9]). The InPd intermetallic's physical characteristics have been studied. In this work, the electrical, thermal, magnetic, and hydrogen-absorption properties of InPd phase single crystals produced using the Czochralski process were determined (Wencka *et al*. [10]).

The electrical and elastic properties of the InPd intermetallic combination have received very little attention, according to the literature currently in publication. This article presents a systematic investigation of the electrical structure and elastic properties of InPd intermetallic. The structural and electrical characteristics of this intermetallic have been investigated using the Quantum Espresso Code. The *Generalised Gradient Approximation* (GGA) in *Density Functional Theory* (DFT) is used to do the current computations for InPd with CsCl structure. The bulk modulus and ground state characteristics are taken into consideration. Additionally, the density of states, band structure computation, and a few elastic properties are investigated. Based on estimated results, it is projected that these intermetallic compounds will be ductile. The following section provides a detailed approach of attainable estimation. In Section 2, the computing procedure is summarised. Section 3 reviews the findings, and Section 4 presents the conclusion.

2. Calculation Method

A computational method for calculating periodic and disordered systems from fundamental principles is called quantum espresso (Giannozzi *et al*. [4]). Its primary foundations are plane waves, pseudopotentials (electron-electron interaction), and DFT theory (electron-ion interaction). It determines the Kohn-Sham orbital and ground state energy for metals and insulators as well as different kinds of structural optimisations. Quantum Espresso is applicable for studying a variety of materials, including semiconductors, metals, and insulators. FPMD

(*First Principle Molecular Dynamics*), CP (*Car Parinello*), and PWSCF (*Plane Wave Self Consistent Field*) are the three main components of the methodology. Irreducible k-points for quantum espresso are constructed using the Monkhorst-Pack approach (Giannozzi and Cavazzoni [3]). To broaden the Kohn-Sham single-particle functions, a plane-wave set was employed with a kinetic energy cut-off of 34 Ry. To acquire a well-converged ground state energy, the Brilliouin-zone was sampled using a $12 \times 12 \times 12$ k-point mesh. The exchange and correlation effects have been discussed by the GGA. The lattice parameter, bulk modulus, and pressure derivative of the bulk modulus were estimated using the standard procedure of computing the total energy for different volumes, and they were subsequently fitted to Murnaghan's equation of state (Murnaghan [8]).

3. Result and Discussion

The equilibrium atomic structure of the crystal is found by minimising the total energy using the first principles pseudopotential (PWSCF) technique.

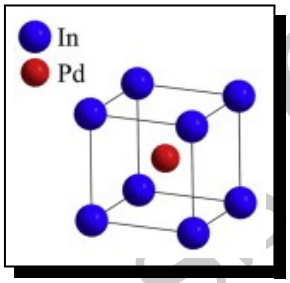

Figure 1. Crystal structure of InPd

The equilibrium lattice constants were determined by minimising the total energy. These parameters were used in the calculations of the non-self-consistent band structure. Fitting these energy values to Murnaghan's equation of state has yielded the equilibrium lattice constant (a), bulk modulus (B), and its pressure derivative (B') at minimal equilibrium volume V_0 (Wencka *et al*. [8]),

$$P(V) = \frac{B}{B'}\left[\left(\frac{V_0}{V}\right)^{B'} - 1\right], \tag{3.1}$$

where the equilibrium volume V_0 and the bulk modulus B are the fit parameters:

$$B = -V\frac{\partial P}{\partial V} = V\frac{\partial^2 E}{\partial V^2} \tag{3.2}$$

and its pressure-dependent derivative, $B' = \frac{\partial B}{\partial P}$. Table 1 lists the calculated structural parameters, which are the pressure derivative of bulk modulus (B'), cohesive energy (E), and lattice constant (a). These criteria are used for comparison of the existing findings. The conclusions presented are obviously in good agreement with recent experimental data (Giovannini *et al*. [5]) and previous theoretical results (Gaudry *et al*. [2]).

Additionally, the electronic properties of InPd are investigated by analysing its electronic *band structure* (BS), *total density of states* (TDOS), and *partial density of states* (PDOS). Accordingly, Figures 2-6 display these electrical properties. Figure 2 depicts the InPd band structure, while Figure 3 shows the total density of states next to the wave vector. It is evident from the hybridisation that the current intermetallic compound has metallic characteristics.

Table 1. Ground state properties of InPd

Intermetallic	Approach	Lattice constant a (Å)	Cohesive Energy E(eV/at)	B'
InPd	Present	3.27	−3.43	1.04
	Experimental	3.25[a]	—	—
	Others	3.30[b]	−3.57	—

[a]: reference [5], [b]: reference [2]

InPd's electronic characteristics are analysed using its electronic *Band Structure* (BS), *Total Density of States* (TDOS), and *Partial Density of States* (PDOS). The band structure reveals the allowed energy states and indicates whether a band gap is present or absent, which is shown in Figure 2 and shows the fluctuation of electron energy with respect to the wave vector in the Brillouin zone. The overall density of states, which measures the quantity of accessible electronic states at every level, is shown in Figure 3. Important details regarding the electrical distribution and the conductive characteristics of the material are revealed when TDOS is analysed in conjunction with the wave vector. One important finding from this analysis is that InPd shows metallic behaviour since the TDOS stays nonzero at the Fermi level.

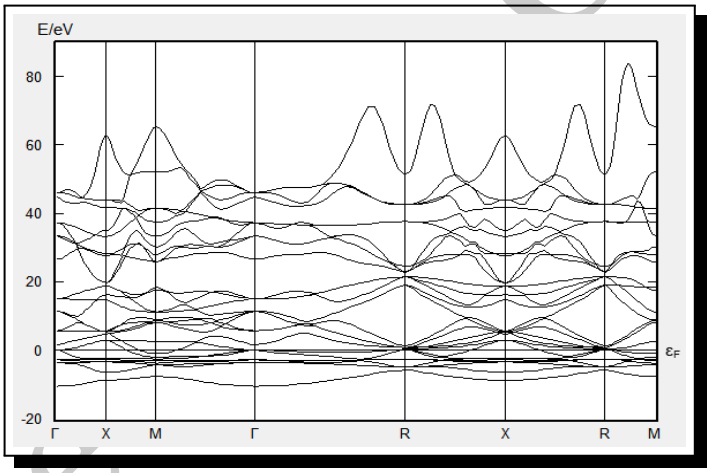

Figure 2. Electronic band structure of InPd in CsCl-phase

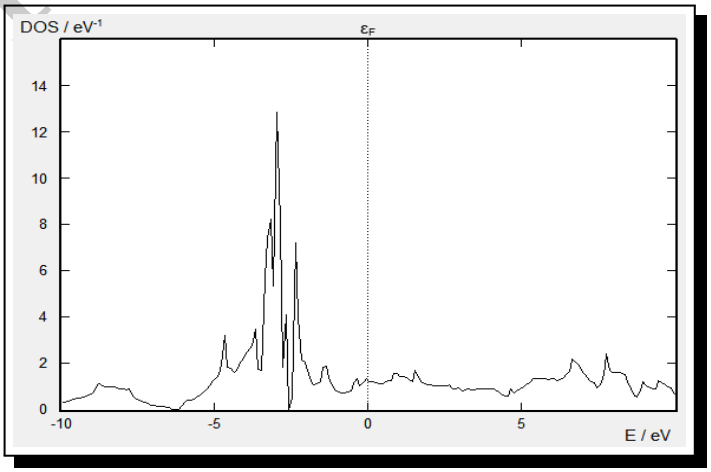

Figure 3. Total Density of State (TDOS) of InPd in CsCl-phase

Furthermore, the PDOS analysis, which is depicted in Figures 4-6, provides a deeper understanding of orbital hybridisation by breaking down the total density of states into contributions from various atomic orbitals. Strong electronic interactions are suggested by the notable hybridisation between the orbitals of *indium* (In) and *palladium* (Pd), which supports the intermetallic compound's metallic character. These hybridised states are found close to the Fermi level, confirming that InPd has free electrons that contribute to electrical conductivity and no band gap. Thus, the metallic properties of InPd are clearly established by the combined study of BS, TDOS, and PDOS, highlighting its potential use in conductive and electrical applications.

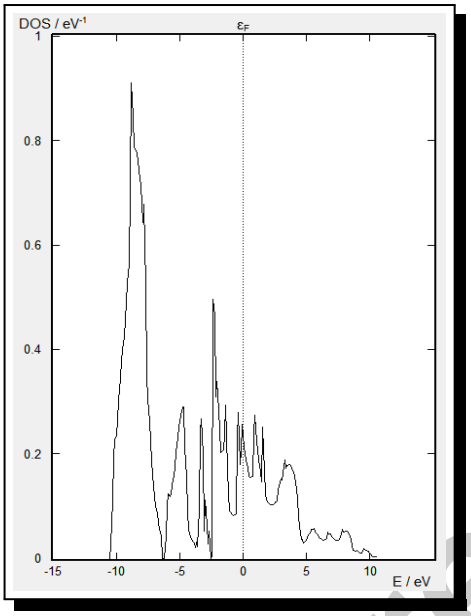

Figure 4. Partial Density of State (PDOS *s*-state) of InPd in CsCl-phase

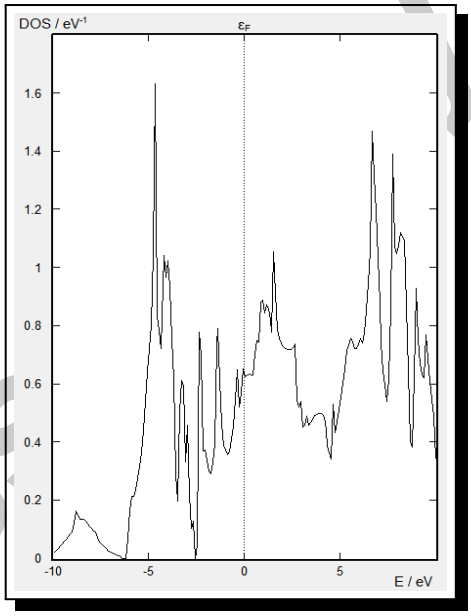

Figure 5. Partial Density of State (PDOS *p*-state) of InPd in CsCl-phase

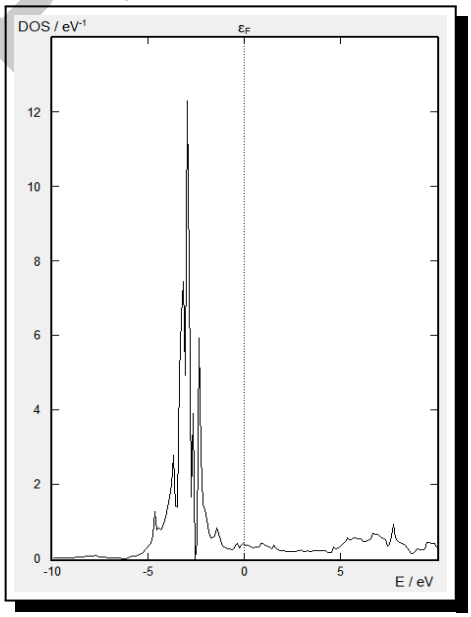

Figure 6. Partial Density of State (PDOS *d*-state) of InPd in CsCl-phase

4. Conclusion

In summary, first-principles computations were employed to explore the structural and electronic behavior of InPd intermetallics. The bulk modulus and lattice parameter, among other structural characteristics, were effectively computed. These parameters agree well with other experimental and theoretical approaches. The current intermetallic compound's metallic nature has been electrically verified.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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