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Density Functional Investigation of Scandium Based $ScIn_3$ Intermetallic Compound in $AuCu_3$ structure

G. Pagare
Department of Physics,
Sarojini Naidu Government Girls P.G. Autonomous College, Bhopal, (Madhya Pradesh), India

(Corresponding author: G. Pagare, gita_pagare@yahoo.co.in)
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ABSTRACT: A theoretical study on structural, electronic and elastic properties of cubic $ScIn_3$ intermetallic, which crystallizes in $AuCu_3$ structure, have been investigate during full-potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory. The generalized gradient approximation and local density approximation is used for exchange-correlation (XC) potential. We have calculated the ground state properties such as lattice constant (a_0 = 4.537Å and 4.3910Å), bulk modulus (B = 55.04GPa and 72.89GPa) and pressure derivative of bulk modulus (B'= 4.97 and 4.96) for $ScIn_3$ using PBE-GGA and LDA respectively. Our calculated lattice constants are in good agreement with the experimental and other theoretical data available. The second order elastic constants (C_{11} = 92.34GPa, C_{12} = 38.71GPa and C_{44} = 15.70GPa) have been calculated using PBE-GGA at ambient condition. The electronic band structure (BS) and density of states (DOS) of this compound, show the metallic nature. Poisson's ratio (σ), Young's Modulus (E), Shear modulus (G_H) and the ratio of anisotropy factor (A) are also reported. Ductility/brittleness of this compound is further analyzed by calculating the ratio B/G_H and Cauchy pressure (C_{12}-C_{44}). The studied compound is found to be ductile in nature.

Keywords: First Principles Calculation, Ab-*initio* Calculation, Elastic constants, Electronic properties.

I. INTRODUCTION

The intermetallic compounds with AB_3 formula are currently under intense investigations due to their structural and physical properties [1]. Scandium-based compound $ScIn_3$ is an intermetallic compound with $AuCu_3$ structure, which belongs to Pm-3m space group. The electronic structure and transport properties of ScX_3 (X= Ga, In) was investigated by FP-LAPW methods by Sharma *et al*. [2]. To the best of our knowledge, there is no systematic report present in light on structural, electronic, elastic and mechanical behavior of $ScIn_3$ intermetallic using FP-LAPW. This motivated us to study of this compound. The paper is organized as follows. The computational methodology is briefly described in section II. Section III deals with the results and discussion of the present work. Finally, section IV presents conclusion.

II. COMPUTATIONAL METHODOLOGY

$ScIn_3$ compound crystallizes in a simple cubic $AuCu_3$ structure with four atoms per unit cell. It belongs to the *Pm3m* space group with Sc atoms occupying the corners of the cube while the In atoms occupying the cube faces. First-principles study of the $ScIn_3$ compound was performed by employing full potential linearized augmented plane wave (FP-LAPW) method [3] based on density functional theory within the generalized gradient approximation (GGA) incorporated in the WIEN2k code [4]. It is a variational method that is at present the most successful approach to compute the electronic structure of matter. The density functional theory is derived from the N- particle Schrodinger equation and useful for system of many electrons. The exchange correlation potential is treated with generalized gradient approximations in the scheme of Perdew, Burke and Ernzhof (PBE-GGA) [5], Wu and Cohen (WC-GGA) [6] and Perdew *et al*. (PBEsol-GGA) [7] to investigate the structural, electronic, elastic, mechanical and thermal properties of $ScIn_3$ compound. The basis function has been expanded up to R_{mt}x K_{max} = 7.0, where R_{MT} is the smallest atomic radius in the unit cell and K_{max} gives the magnitude of the largest k vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is l_{max} = 10 while the charge density is Fourier expanded up to G_{max} = 12. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1000 k points and the tetrahedral method [8] have been employed for the Brillouin zone integration.

The total energies are fitted to Birch equation of state [9] to obtain the ground state properties. The elastic moduli require knowledge of the derivative of the energy as a function of the lattice strain. It is well known that a cubic system has only three independent elastic constants namely C_{11}, C_{12} and C_{44}. Hence, a set of three equations is needed to determine all the constants. The first equation involves calculation of bulk modulus (B), which is related to the elastic constants as

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \quad \ldots(1)$$

Where C_{11} and C_{12} are second order elastic constants.

III. RESULTS AND DISCUSSION

We have calculated the ground state properties of $ScIn_3$ in non-magnetic state using first principles FP-LAPW method. The calculated total energies are fitted to the Birch equation of state to determine the ground state properties like lattice constant (a_0), bulk modulus (B) and its pressure derivative (B′) which are listed in Table 1 and compared with the available experimental results. It is seen from Table 1 that our calculated values of a_0 using GGA and LDA are in good agreement with the experimental results. Neither experimental nor theoretical results of B and B′ are available for$ScIn_3$, so we could not compare our results with other measured or theoretical values.

Table 1: Calculated ground state and electronic properties of $ScIn_3$.

Solids	Approx.	a_0 (Å)	B (GPa)	B′ (GPa)	N(E_f) States/eV
ScIn3	PBE-GGA	4.537	55.04	4.97	2.98
	WC-GGA	4.455	65.05	5.01	
	LDA	4.391	72.89	4.96	
	Exp.	4.477[a]			

[a]Ref[10]

The self consistent non-spin polarized electronic energy band structure for $ScIn_3$ intermetallic compound along the high-symmetry directions in AB_3 phase is obtained using FP-LAPW method within PBE-GGA at ambient pressure, and presented in Fig. 1(a). The Fermi level E_F is fixed at the origin. It can be seen that there are some bands cross the Fermi level, which indicates the metallic behavior of $ScIn_3$. The density of states is also plotted in Fig. 1(b). The lowest lying band is mainly due to the '*s*' like state of In, nearly -5 eV and do not contribute much to bonding. Many small peaks are observed in the valence bands in the energy range -5 eV to 0 eV only due to '*d*' like states of Sc. The metallicity at the Fermi level is observed due to the joint contribution of Sc '*d*' and '*s*'and '*p*' states of In but there is major participation of '*d*' like state of Sc. The finite DOS value at Fermi level is obtained as 2.98states/eV. Hence the compound has obvious metallic character.

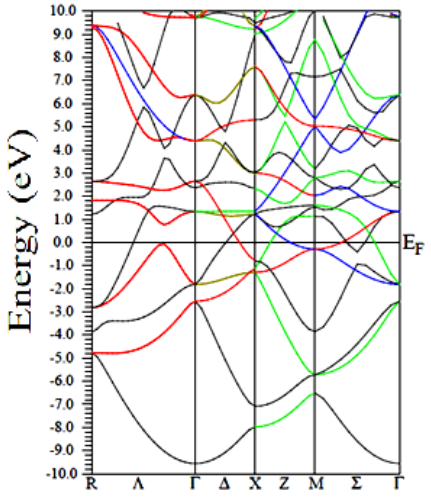

Fig. 1(a) Band structure of $ScIn_3$.

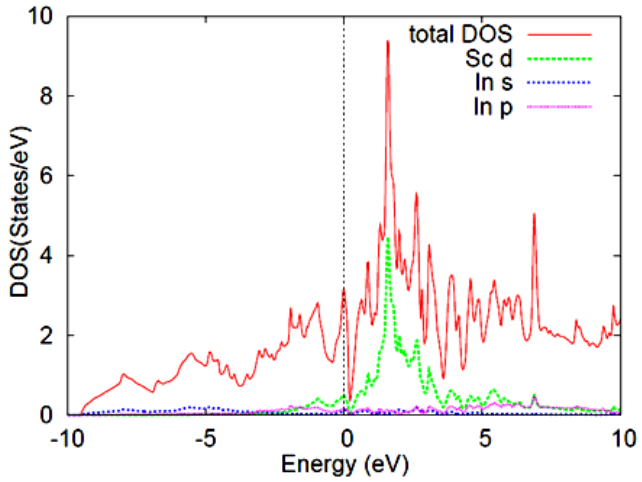

Fig. 1(b) Density of States of $ScIn_3$.

The elastic constants provide a link between the mechanical and dynamical behavior of crystal. We have calculated the elastic constants for $ScIn_3$ using PBE-GGA at ambient pressure using the method developed by Thomas Charpin and integrated it in the WIEN2k package. The calculated values of elastic constants at ambient pressure are given in Table 2. We have also analyzed the ductility of the investigated compound using Pugh's criteria [11] and Cauchy's pressure. If the value of B/G_H ratio is greater than 1.75, the investigated compound is predicted as ductile in nature otherwise it is reported as brittle. Our calculated result indicates that the studied compound is ductile in nature with B/G_H ratio as 2.90. The ductile nature of $ScIn_3$ can also be correlated to the positive Cauchy pressure and thereby metallic nature of the studied compound. It can be noted that our calculated elastic constants satisfy the stability criterions: $C_{11}- C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{12} < B < C_{11}$, which clearly indicate the stability of $ScIn_3$ in $AuCu_3$ structure.

Table 2: Calculated elastic properties of $ScIn_3$.

Solids	Approx.	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B/G_H	C_{12}-C_{44}
ScIn3	PBE-GGA	92.34	38.71	15.70	2.90	23.01

Elastic constants can be used to determine mechanical properties such as Young's modulus (*E*), shear modulus(G_H), Poisson's ratio (σ), and anisotropic factor (*A*) for useful applications. These are fundamental parameters which are closely related to many physical properties like internal strain, thermo elastic stress, sound velocity, fracture, toughness etc.

We have calculated these properties of $ScIn_3$and presented in Table 3. The calculated value of Poisson's ratio reveals the metallic nature of the studied compound. Neither experimental nor theoretical results of these properties are available for $ScIn_3$, so we could not compare our results with other measured or theoretical values.

Table 3: The calculated mechanical properties of $ScIn_3$ at ambient pressure using PBE-GGA.

Solids	E	G_H	σ	A
$ScIn_3$	52.43	19.48	0.34	0.58

IV. CONCLUSION

In conclusion, the structural, electronic, elastic and mechanical properties of $ScIn_3$ have been systematically studied using the FP-LAPW method on density functional theory, within three different forms of generalized gradient approximation (PBE-GGA and WC-GGA) and LDA as the exchange correlation potential. The electronic properties of this compound is studied by calculating the band structures and its corresponding density of states. The calculated elastic constants (C_{11}, C_{12} and C_{44}) have shown that $ScIn_3$compound is elastically stable in the $AuCu_3$ structure. Using these elastic constants, Young's modulus (E), shear modulus (G_H), Poisson's ratio (σ) and anisotropic ratio (A) are also reported. In the present study we found $B/G_H > 1.75$ and $C_{12}–C_{44} > 0$ for $ScIn_3$compound, which implies that this compound is ductile in nature. Our calculated elastic constants obey the necessary mechanical stability conditions for cubic crystals. We report the mechanical properties of this compound for the first time. This will be tested in the future experimentally and theoretically.

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