BAOJ Nanotechnology

Akel O, et al., BAOJ Nanotech 2019, 5: 1
5: 020

Review article

Study of Structural, Elastic, and Electronic Properties of the Ternary Intermetallic ScAuSn

Akel O[1*], Abbar B[1], Cherid S[2] and Benidris M[3]

[1]*Modelling and Simulation in Materials Science Laboratory, Djillali Liabès University of Sidi Bel-Abbès, 22000 Sidi Bel-Abbes, Algeria*

[2]*Laboratoire de structure, Elaboration et applications des matériaux Moléculaires, Faculty of Sciences and Technology, Abdelhamid Ibn Badis University, BP 227, Mostaganem 27000, Algeria*

Abstract

In this paper, we study the structural, elastic and electronic properties of the ternary intermetallic ScAuSn is presented by using the full-potential linearized augmented plane wave (FP-LAPW) method within the generalized gradient in the frame of the density functional theory. We have evaluated the ground-state quantities such as lattice parameter, bulk modulus and their pressure derivatives as well as the elastic constants are calculated to investigate stability criteria and the mechanical nature of the experimental to calculate the phonon dispersion using the plane-wave pseudo potential method. Both compounds are found to be mechanically anisotropic, brittle and meet the elastic stability criteria. Also, we have presented the results of the electronic band structures show a metallic-like character. Our electronic density of states results suggest that the main contributions to the density of states at the Fermi level come from the Sc-3d states, these results were in favorable agreement with previous theoretical works and the existing experimental data.

Keywords: Intermetallic Compound; Density Functional Theory; FP-LAPW; Phase Stability

Introduction

The ternary intermetallic RTX-type compounds (where, R are rare-earths, T are 3d- transition metals, X p-elements) crystallize in numerous types of structure. However, the CeFeSi (P4/nmm), TiNiSi (Pnma) and ZrNiAl (P−62m) structures types, have been the most studied during the last years.

The configuration of RAuSn was first reported by Rossi et al. [1] and Mazzone et al. [2] who also determined their crystal structures. Most of the RAuSn compounds are used in electronic circuits [3]. Several theoretical and experimental works have been done on the structural, electronic and optical properties of these materials [4–5]. The magnetic and transport measurements on RAuSn compounds have been studied by different experimental groups [6-7]. Recently ScAuSn, YAuSn and LuAuSn have been synthesized and their various physical properties such as crystal data, structure refinement, and magnetic susceptibilities have been reported by Sebastian and al [8].

Fixing elastic properties is important for determining the mechanic response of the structure to external constraints; the evaluation of the bulk and shear modulus informs us on the materials strength and their hardness, it is obviously for all these reasons that we will calculate the pressure effect on elastic constants of the ScAuSn compounds. The aim of the present work is to investigate structural and electronic properties of ScAuSn by using the full-potential linearized augmented plane wave (FP-LAPW) method within the generalized gradient approximation (GGA) within the framework of density functional theory (DFT), and compared with those obtained by the application of the plane-wave pseudo potential method by F. Soyalp and S. Ugur [12].

***Corresponding Author:** Akel Omar, Modelling and Simulation in Materials Science Laboratory, Djillali Liabes University of Sidi Bel-Abbes, 22000 Sidi Bel-Abbes, Algeria, E-mail: akel.omar@hotmail.com

Sub Date: January 18th 2019 **Acc Date:** February 4th 2019, **Pub Date:** February 8th 2019

Citation: Akel O, Abbar B, Cherid S, Benidris M (2019) Study of Structural, Elastic, and Electronic Properties of the Ternary Intermetallic ScAuSn. BAOJ Nanotech 5: 020.

Models and Computational Aspects

ScAuSn is known to crystallize with the well-known F-43m space group, with three atoms per unit cell. In this work, the electronic structure and the basic ground state properties of the ScAuSn intermetallic alloys are calculated using the full potential linearized augmented plane-wave (FP-LAPW) method implemented in the WIEN2k calculation code [9–10]. The crystalline structures of both alloys are presented on Figure 1. As shonw, they are of a cubic phase. The three atoms have coordinates τSc=(1/2,1/2,1/2), τAu=(3/4,3/4,3/4), τSn=(0,0,0).

The PWs cut-off was used with the highly recommended condition RMTKmax = 8.5, where RMT is the average of the muffin-tin spheres and Kmax is the PW cut-off. The sphere radii used in the calculations are 2.4, 2.5 and 2.47 a.u. for Sc, Au and Sn, respectively. The k-space integration over the Brillouin zone was performed using a mesh of 56 k-points of the irreducible part in the Brillouin zone.

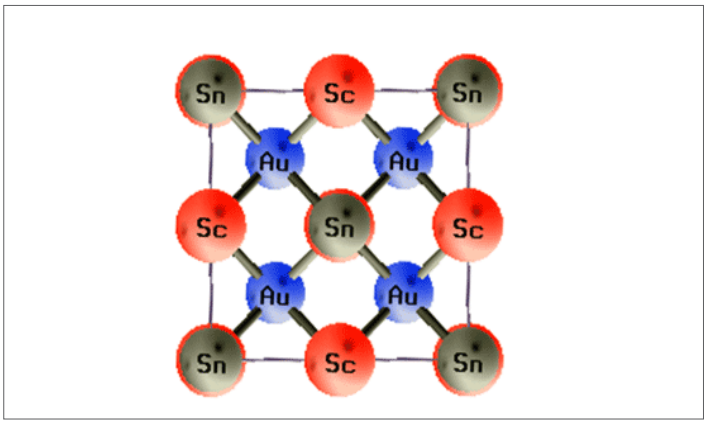

Figure 1: Crystalline structures of ScAuSn F-43m space group

Results and Discussion

Structural Properties

All physical properties are related to the total energy. For instance, the equilibrium lattice constant of a crystal is the lattice constant that minimizes the total energy. If the total energy is calculated, any physical property related to it can be determined as shown in Figure 2

In this section, we present the results of structural properties for ScAuSn compounds. To obtain the equilibrium lattice constant and determine the stable structure of these alloys, we perform a non-magnetic phase (NM) optimization calculations ScAuSn alloys first, using GGA approaches. The calculated total energies versus volume are fitted with the empirical Murnaghan's equation of state [11] to determine the ground state properties. Our work yields a lattice constant of 6.522 Å, in agreement with the experimental value of 6.419 Å [8] to within 1.60 %, and that calculated by the use of The plane-wave pseudo potential method (6.501 Å) [12].

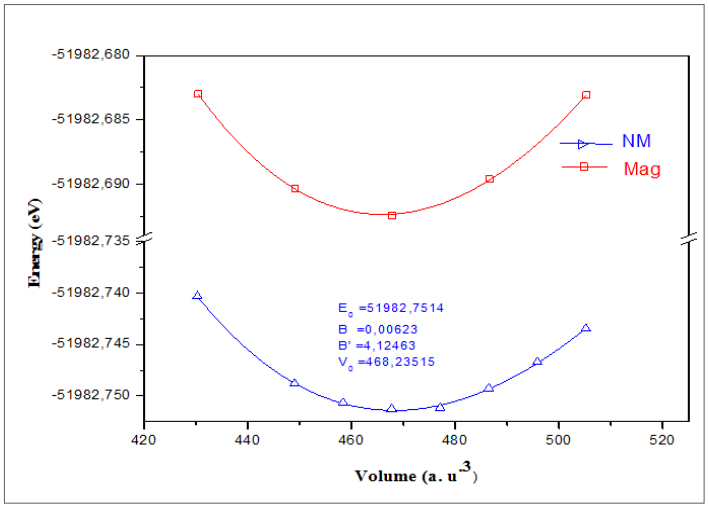

Figure 2: Comparison of the structural stability ScAuSn compounds, using GGA approaches

Table 1 : Calculated equilibrium lattice constant (a) (Å), cell volume V0 units (a.u.3), Minimum energy E (Ry), bulk modulus B (GPa) with its pressure deriv ative B' for ScAuSn compounds, compared to available data : ils ont pas bien structurer

Material	Ref	V_0 (a.u.^{3})	E_0 (Ry)	a (Å)	B (GPa)	B'
ScAuSn	This work	468.2336	-51982.7514	6.5229	123,088	4.13
	Ref.[12]	-	-	6.501	-	4.02
	Ref.[8]	-	-	6.419		-
Ref.[8] Exp.						
Ref.[12] Theo.						

Elastic Properties

The elastic constants describe the response of a system to an applied macroscopic stress. The knowledge of these constants is important, because they are directly employed in practical uses of materials. Various experimental techniques are available for the measurement thermodynamic stability such as the full phonon-dispersion curves are necessary for a microscopic understanding of the lattice dynamics. The knowledge of the phonon spectrum plays a significant role in determining various materials properties.

The calculated elastic constants at P = 0 and T = 0 are listed in Table 2, Considering the cubic lattice, there are only three independent elastic constants C_{11}, C_{12} and C_{44}, the shear modulus G, the B/G ratio, the Young's modulus E, the Poisson's ratio (υ), the Zener anisotropy factor (A), the densities (ρ), the longitudinal elastic wave velocities V_l, the transverse elastic wave velocities Vt, the average acoustic velocity Vm, and the Debye temperature (θD) of ScAuSn compounds.

The mechanical stability requires that C_{11}- $C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$ and $C_{12} < B < C_{11}$, C_{11}- $C_{12} > 0$ [13] . For ScAuSn the elastic constants satisfy these stability conditions, indicating that the cubic structure is a mechanically stable phase.

The obtained elastic constants are used to compute the anisotropy constant [14], which is given by the relation $A = 2C_{44}/(C_{11} - C_{12})$ we obtain the anisotropy parameter

A =1.28. This indicates that the elastic properties are highly anisotropic. The shear modulus G represents the resistance to plastic deformation, according to Hill [15], the Voigt [16] and Reuss [17] expressions represent the upper and lower limit for the polycrystalline crystals, respectively, and the arithmetic mean value can then be taken for estimation of the shear modulus.

In order to predict the brittle and ductile behavior of materials, Pugh [18] proposed an approximate criterion by the ratio of B/G. Higher (lower) B/G ratio corresponds to ductile (brittle) behavior. The critical value that separates brittle and ductile materials is about 1.75. The data in the Table 2 indicate that the B/G ratio is 1.37, suggesting that ScAuSn alloys are brittle. The Poisson's ratio calculated value confirms the ductile nature of these compounds. Indeed, for a brittle material, the Poisson's ration υ must be lower than 1/3, otherwise the material confirmed is brittle. The value of the Poisson's ratio can also indicates the degree of directionality of the covalent, ionic or metallic materials. The latter obtained for ScAuSn is 0.207, which is an indication that the inter-atomic forces are central forces [19].

The Young's modulus E is very important in technological and engineering application [20]. It is the usual property used to characterize stiffness, such a way, the higher the value of E, the stiffer is the material. According to our investigations, the ScAuSn alloy is found to be stiffer.

Table 2: Calculated elastic constant C_{11}, C_{12}, and C_{44} shear modulus G, ratio of B/G, Young's modulus E, Poisson's ratio **υ,** Zener anisotropy factor A, density **ρ**, longitudinal elastic wave velocities V_l, transverse elastic wave velocities V_t, average acoustic velocity V_m, and Debye temperature (θ_D) for ScAuSn

Compounds	C_{11}(GPa)	C_{12}(GPa)	C_{44}(GPa)	B/G	G(GPa)	E(GPa)	υ
ScAuSn	197.683	84.791	71.94	1.37	65.05	157.15	0.207
Compounds	ρ(g/cm³)	V_l(m/s)	V_t(m/s)	V_m (m/s)		θ_D (K)	A
ScAuSn	8.638	4519.093	2744.143	3032.087		316.842	1.28

Electronic Properties

Band structure: Density of states and electronic band structure often provide sufficient information for a thorough characterization of the electronic properties of a material. The calculated band structures of the ternary intermetallic ScAuSn compound at equilibrium lattice constants along the higher symmetry directions in the Brillouin zone as shown in Figure 2. It can be seen the intersection of the bands with the Fermi level, the band structures for all compounds exhibit a gap separating the anion and the cation states, while the bands are strongly metallic.

The experimental values, in which EF = 0 is taken, shows the electronic band structure of ScAuSn along the several symmetry directions [12]. The calculated Γ–Γ, X –X and Γ –X bands gaps are 1.40, 1.48 and 0.07 eV, respectively. The one band cross the Fermi level along the K–X–Γ and L–X–W directions. ScAuSn is an almost zero indirect band gap, and a small direct transition at the X-point. This picture clearly indicates the metallic nature of this material.

Density of States (DOS): The calculated density of states (DOS) on Figure 3. shows the total and partial electronic states densities for sub-bands of nonmagnetic ScAuSn compounds F-43m space group intermetallic types. The variations of ScAuSn density of states are similar to that of the band structure; however, the magnitudes and the positions of the peaks are the same. We distinguish three main regions: the peak at the lowest energy states (≤ - 3 eV) , which is merely due to the localized electrons s- of Sn, while the next region between 0 and -3 eV contains the contribution of ***p***- states of Au and

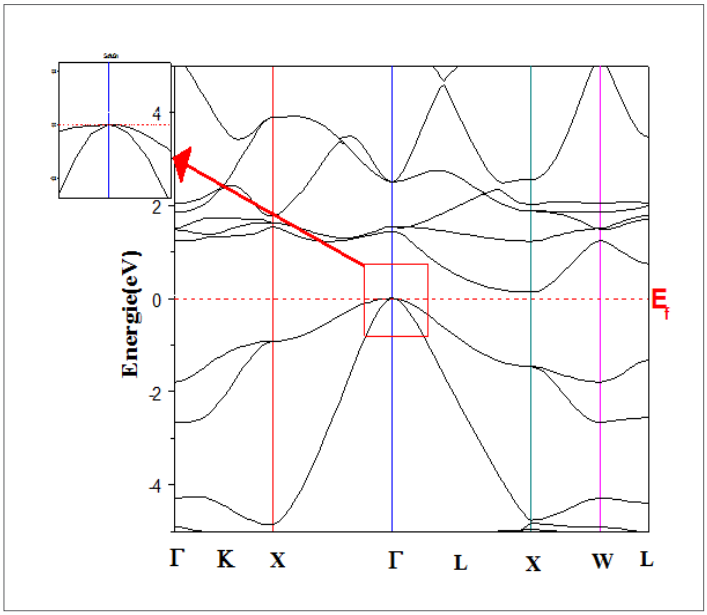

Figure 3: Band structures for: ScAuSn. The Fermi level is indicated by the horizontal line at zero energy.

Sn. The conduction-band is predominately ***d***- states of Sc with only a small contribution from ***p***- and ***s***- states of Sn. A wide band formed by ***d***-states of Sc due to hybridization is much extended in energy and is characterized by high intensity. This main discordance comes from the fact that we use in our work a different approximation (GGA), implanted in a different calculation code. In all cases, the general aspect is maintained. Furthermore, all total states densities confirm

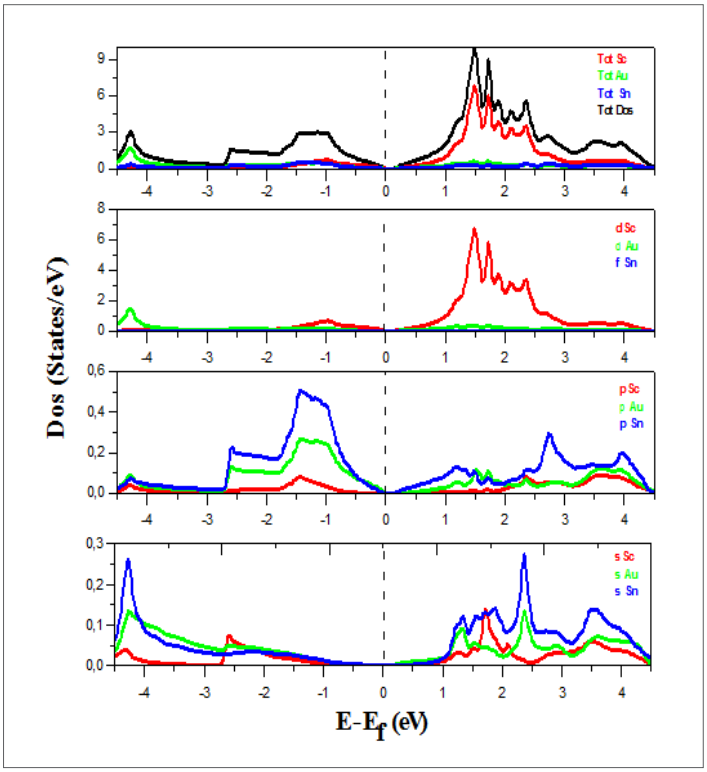

Figure 4: Total and partial densities of states (PDOS) of the ScAuSn, obtained by GGA.

the metallic behavior of our structures.

Conclusions

In this paper, using the FP-LAPW, we have presented an analysis of the structural, elastic, and electronic properties of ScAuSn, the calculated structural properties obtained by GGA approximation (equilibrium lattice constant, bulk modulus and its pressure derivative) are in good agreement with values reported in the literature. The elastic constants C_{11}, C_{12} and C_{44} were obtained from calculations but need to be confirmed in the future due to lack of experimental data. This ternary intermetallic alloy is mechanically stable according to the elastic stability criteria and shows ductile behavior; hence our results were only compared with the available theoretical values. Electronic properties investigations of these materials lead to band structures and densities of states revealing a metallic nature.

The reported calculations provide new structural, elastic, and electronic results for ScAuSn Hence; this study forms part of a large

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