A first principles study on the orthorhombic $ScNiAl_3$

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ABSTRACT

We have used to ab-initio methods for determining the structural, electronic, and elastic properties for the $ScNiAl_3$ compound in orthorhombic Pnma structure (Spg No:62). The pseudopotential plane-wave approach is used based on density functional theory and implemented in the VASP package. We have computed the basic physical parameters such as lattice constants, bulk modulus, elastic constants. The elastic constants are calculated using stress-strain relationship and their corresponding elastic moduli of polycrystalline aggregate, including shear moduli (G), Young's moduli (E), Poisson's ratios (v), and elastic anisotropy values (A) are obtained. The electronic band structures, total and partial density of states of these materials are given. The calculations reveal that $ScNiAl_3$ is mechanically stable and have a soft-ductile nature metallic compound.

1. INTRODUCTION

There are a large number of studies about R-Ni-Al systems, where R is a rare earth metal, because of their glass-forming ability [1, 2]. This system belongs many structures of these aluminides with different stoichiometry [1]. Pukas et al. were synthesized by arc melting of $RNiAl_3$ (R = Y, Sm, Gd, Tb, and Dy) compounds. Theirs x-ray diffraction study show that these compound crystallize with $YNiAl_3$-type structures (SPG Pnma, No: 62) [1]. The structural and physical properties of $ScNiAl_3$ compound, same group element of $YNiAl_3$, don't know, yet. In this study, we have performed the first principles structural and mechanical calculations for the first time.

2. METHOD

All calculations have been carried by using the VASP code [3-4] based on the density functional theory (DFT). The electron–ion interaction was considered in the form of the projector-augmented-wave (PAW) method with plane wave up to an energy of 500 eV [5], an adequate value for studying the physical properties. Perdew–Burke–Ernzerhof (PBE) type functional [6] within the generalized gradient approximation (GGA) has been used for the exchange and correlation terms in the electron–electron interaction. 6x11x4 Monkhorstand Pack [7] grid of k-points has been used. The stress-strain method, implemented in the VASP code, was used to predict the second order elastic constants [8].

3. RESULTS AND DISCUSSION

3.1. Structural properties

$ScNiAl_3$ compound is considered in the orthorhombic Pnma structure (Space Group No:62, Z=4) [1]. The structural view of the titled compound is given in Fig. 1. The experimental structural parameters of $YNiAl_3$ were used as an input for structural energy minimization. The calculated lattice parameters, ground state energy E_0 and volume are listed in Table 1. There is no information on structural parameter of the titled compound, but our results are compatible with prototype compounds' data.

Table 1. The calculated lattice parameters a (Å), b (Å), c (Å), energy E_0 (eV/f.u.), volume V_0 ($Å^3$/f.u.) for $ScNiAl_3$ compound in orthorhombic Pnma structure

a	*b*	*c*	*E_0*	*V_0*	*Ref.*
8.019	3.929	10.393	-25.64	81.88	Present
8.1532	4.0426	10.6349			Exp.[1] for $YNiAl_3$

3.2. Electronic properties

We were calculated the electronic band structure of $ScNiAl_3$ compound and given in Figure 2. It can be seen from the figure that this compound has metallic nature. From Fig. 2, while valence band electrons originate from Ni atoms, but conduction band electrons are from Sc atoms.

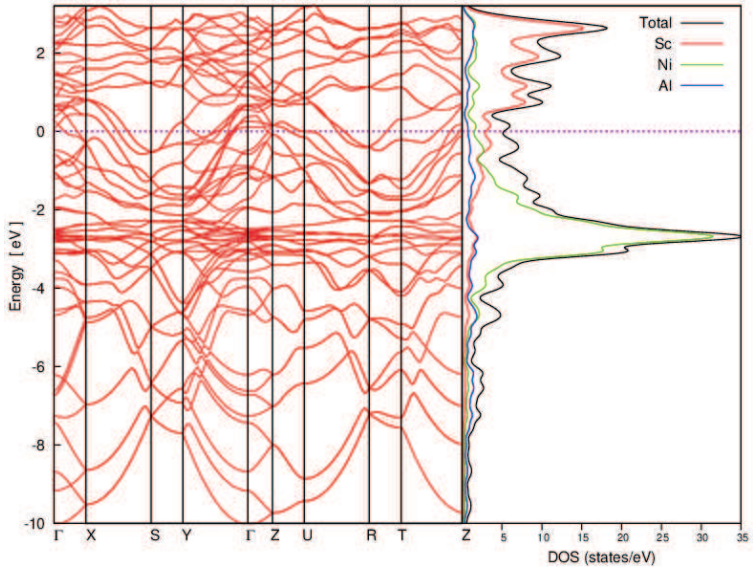

Figure 2. The calculated electronic band structure and partial density of states of $ScNiAl_3$

3.3. Mechanical properties

"Stress-strain" method [8], implimented in VASP, were used to compute the second order elastic constants (C_{ij}), and the findings are given in Table 2. The Born's mechanical stability criteria for orthorhombic systems are given below [9-11];

- $C_{11} > 0$, $C_{22} > 0$, $C_{44} > 0$, $C_{33} > 0$, $C_{55} > 0$, $C_{66} > 0$
- $C_{11} + C_{22} > 2C_{12}$
- $C_{22} + C_{33} > 2C_{23}$
- $C_{11} + C_{33} > 2C_{13}$
- $C_{11} + C_{22}C_{33} + 2C_{12} + 2C_{23} + 2C_{13} > 0$

Our results for elastic constants are given in Table 2 satisfy these stability conditions means $ScNiAl_3$ compound mechanically stable in the considered phase.
The mechanical properties, such as bulk modulus (B), Young's modulus (E), shear modulus (G), Poisson's ratio (v) and shear anisotropy factors (A) which are functions of the elastic constants, are calculated by using the Voigt–Reuss–Hill approximation [12, 13], and are tabulated in Table 3.

Table 2. The calculated elastic constants (C_{ij} in GPa unit).

C_{11}	C_{12}	C_{13}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}
184.5	59.1	61.0	159.6	78.4	160.3	33.5	77.8	64.1

Table 3. Calculated bulk modulus (B in GPa), isotropic shear modulus (G in GPa), Young's modulus (E in GPa), Poisson's ratio (v), B/G ratio, Shear anisotropiy factors (A_1, A_2, and A_3), the percentage of anisotropy in the compression and shear (A_B, A_G in %),

B	G	E	v	B/G	A_1	A_2	A_3	A_B	A_G
100.1	52.9	134.9	0.27	1.89	1.39	0.82	1.13	0.01	4.77

According to criterion, a material is brittle (ductility) if the B/G ratio is less (high) than 1.75. The calculated value of the B/G (1.89) is high than 1.75 for the titled compound; hence, the compound will behave in a ductile manner. The typical value of Poisson's ratio is about v = 0.1 for covalent materials and 0.25 for ionic materials. In the present case the value of v is 0.27 for $ScNiAl_3$. Thus, the ionic contributions to the atomic bonding are dominant for $ScNiAl_3$.

For a completely isotropic material, the factor *A* takes the value of 1. When the value of *A* is smaller or greater than unity, it is a measure of the degree of shear anisotropy. The results show that the compound has shear anisotropy.

We also visualize and calculate the directional dependence of the Young's modulus, linear compressibility, Shear modulus, and Poisson ratio by using ELATE code [14, 15]. In the plots of these physical properties, the degree of anisotropy is indicated by the deviation from the spherical shape. These parameters along the crystallographic directions (in 3D) have been given in Fig. 2 for $ScNiAl_3$ compound.

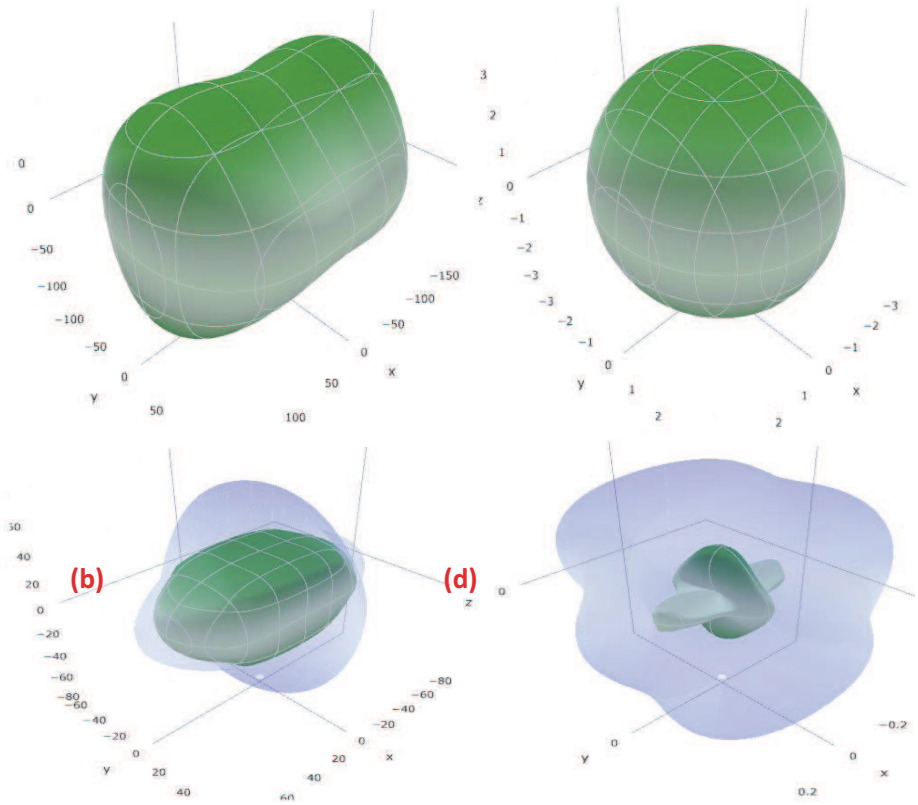

Figure 2. The calculated 3D directional dependence of the mechanical properties; Young's modulus (a), linear compressibility (b), Shear Modulus (c), Poisson's ratio (d) for $ScNiAl_3$ compound.

According to Fig. 2, Young's modulus, Shear modulus and Poisson's ratio exhibiting elastic anisotropy along directions. But, linear compressibility (see Fig. 2b) do not change with directions. This results support the calculated A_G value (in Table 3) is nearly zero.

4. CONCLUSION

In summary, we have performed the first principles total energy calculation for orthorhombic $ScNiAl_3$ compound using the PAW-PP approach and DFT within the generalized gradient approximation. The $ScNiAl_3$ solid, which did not have any experimental study, was similar to the other existing structures. We have revealed that the band structure of this compound is metalic in nature. The B/G ratio is 1.89 and the ductile character is dominant. $ScNiAl_3$ has elastic anisotropic character except for bulk modulus. We hope that our other predicted results will be serving as a reliable reference for the future experimental and theoretical studies.

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