The Electronic, Thermal and Superconducting Properties of V_3Au Intermetallic Compound: An *Ab Initio* Study

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Abstract- **The electronic and superconducting properties of A15 superconducting compound namely, V_3Au have been studied through electronic structure computations by using the first principle tight-binding linear muffin-tin orbital (TB-LMTO) method within atomic sphere approximation (ASA). The electronic and superconducting properties like electronic density of states, energy band structure, Fermi energy, Debye temperature, Gruneisen constant, electronic specific heat coefficient, electron-phonon coupling constant and transition temperature of the material have been studied in terms of Wigner-Seitz cell volume. The total energy as a function of volume has been studied for the compound and equilibrium lattice parameter and bulk modulus have been obtained. The calculated values are compared with the available literature data.**

***Key words*: TB-LMTO; Band structure; Density of states; Debye temperature; Electron-phonon coupling constant; Superconductivity.**

I. INTRODUCTION

The first studies on the binary inter metallic compounds of A15 family have been intensively investigated [1-3]. The superconductors with the A15 structure and A_3X composition generally show very interesting superconducting properties like high critical fields and temperatures. The high temperature superconductors of A15 structure are also known to be strong electron-phonon coupling materials [4]. The fascinating physical properties observed in this material motivate us to carry out the present *ab initio* studies of electronic and superconducting properties. The above interesting electronic and other properties of V_3Au requires detailed knowledge of their fundamental electronic properties such as electronic band structure, electronic density of states, electronic total energy and superconducting properties.

II. MATERIALS PROPERTIES

The A15 materials have high transition temperature and high critical current values [5]. The stability of the A15 compounds is directly related to their electronic structures and more precisely to the structure of their *d*-bands [6]. High-quality, large single crystals of the A15 compounds are necessary in a variety of physical properties studies such as investigations of band structure and lattice disorder. The resistivity $\rho(T)$ of V_3Au shows a T^2 dependence [7] at low-temperatures.

III. COMPUTATIONAL DETAILS

The space group of V_3Au is Pm-3n (no.223). The atomic position in V_3Au is V: ¼, 0, 1/2, and Au: 0, 0, 0. The band structure calculations for the vanadium compound have been carried out by using the tight-binding-linear-muffin-tin-orbital method within the atomic sphere approximation [8]. The density of states has been computed by the method of tetrahedron [9]. The k-mesh in the irreducible wedge of the Brillouin zone of V_3Au has 20 irreducible k-mesh points from a total number of 216 (6x6x6) points. The basis set included *s*-, *p*-, *d*- and *f*-orbitals. The ground-state properties were calculated for the lattice parameter that corresponds to the minimum of the total energy. The following basis set was used for the calculations: V: [Ar] $3d^3 4s^2 p^0$, Au: [Xe] $4f^{14}$ $5d^{10}$ $6s^1$

IV. RESULTS AND DISCUSSION

The plot of total energy as a function of volume in the case of V_3Au is shown in Figure 2. The lattice constant and bulk modulus by fitting the total energy versus volume according to the Murnaghan's equation of state [10].

$$E_T(V) = V\,\frac{B_0}{B_0'}\left[\frac{\left(V_0/V\right)^{B_0'}}{B_0'-1}+1\right] + \text{const.} \qquad (1)$$

where B_0 is bulk modulus and B'_0 is the pressure derivative of B_0. The equilibrium lattice constant is obtained by computing total energies by varying the cell volume of V_3Au compound. The minimum energy value corresponds to the volume and corresponding lattice constant of V_3Au is obtained using TB-LMTO method. The calculated lattice parameter is 4.8082 (Å). It is good agreement with the experimental value 4.8740 (Å) [9].The variation of the lattice constant is in compliance with the variation of the size of atoms in the compound.

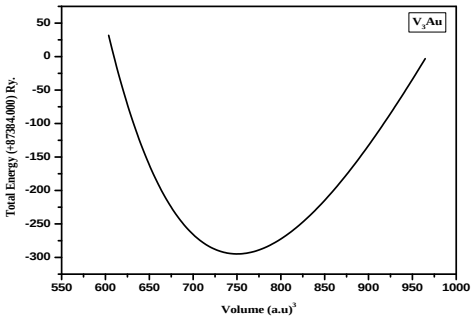

Figure 1. Total Energy *vs* Volume for V_3Au

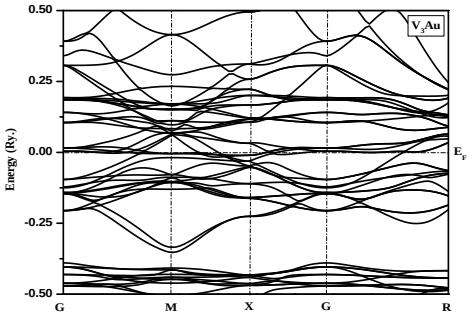

Figure 2. Band structure of V_3Au along symmetry directions

The Fig. 3 has shown the plots of energy bands of V_3Au. The domination of *d*- and *p*-bands is clearly evident in the material. They are also very strongly hybridized. Highly dense accumulation of *p*- and *d*-bands occurs around the Fermi energy for the compound.

TABLE 1. ELECTRONIC DENSITY OF STATES AT THE FERMI ENERGY FOR V_3AU

Bands	**DOS at E_F ((states/Ry)/cell)**			
	V_3Au			
	V	*Au*	*E*	*Total*
s	0.4	0.04	0.9	1.3
p	5.7	4.6	0.5	10.8
d	88.0	7.9	-	95.9

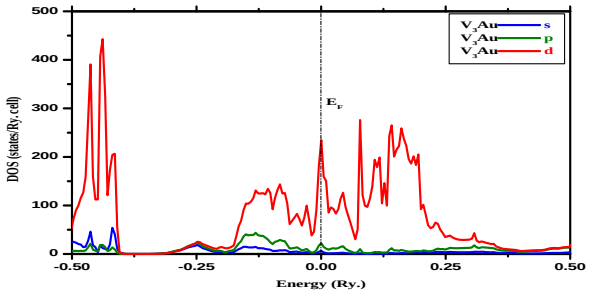

Figure 4. Partial density of states at Fermi level for V_3Au

The Figure 4 shows that the total and partial densities of states of V_3Au compound. It can be seen that *d*-states dominated the DOS of the intermetallic compound over all contribution from *s*-, *p*-, and *f*- states. The DOS at the Fermi level is almost exclusively of *d*- character. The DOS at E_F for V_3Au is presented in Table 1.

The Debye temperature (Θ_D) and Gruneisen constant (γ_G) are important parameters and are closely related to the thermal properties of materials. To calculate the thermal properties of a vibrating Debye lattice we have used the Debye - Gruneisen model [11, 12]. In the present work, the Debye temperature is calculated using the equation.

$$\Theta_D = 67.48\sqrt{\frac{r_0 B_0}{M}} \tag{2}$$

where r is the Wigner-Seitz radius in a.u., r = r_o (at equilibrium), B_0 is the bulk modulus in kbar and M is the average atomic weight. The Gruneisen constant (γ_G) is related to the Debye temperature (Θ_D) and the volume of the unit cell (V) by the relation [13].

$$¥_G = \frac{\partial \ln \Theta_D}{\partial \ln V} \tag{3}$$

The electronic specific heat coefficient (γ) in (4) is related to the density of states $N(E_F)$ and the electron phonon mass enhancement factor (λ) using the expression (5) [14].

$$¥ = (1+ª)\frac{1}{3}®^2 k_B^2 N(E_F) \tag{4}$$

where k_B is the Boltzmann constant. The calculated values of Θ_D, γ_G, and γ are shown in Table 2. The Debye temperature and the electronic specific heat coefficient (γ) are found to agree reasonably well with the existing experimental reports [15].

TABLE 2 EQUILIBRIUM WIGNER-SEITZ RADII (R_0), BULK MODULII (B_0), DEBYE TEMPERATURE (Θ_D), GRUNEISEN CONSTANT (Γ_G) AND ELECTRONIC SPECIFIC HEAT COEFFICIENT (Γ) FOR V_3AU

Compound	**r_0 (a.u)**	**B_0 (GPa)**	**Θ_D (K)**		**γ_G**	**γ (mJmol^{-1}K^{-2})**	
			Present	*Expt.*	*Present*	*Present*	*Expt.*
V_3Au	2.3385	222.2	260	329 [15]	1.92	13.48	13.08 [15]

$$ª = \frac{N(E_F)\langle I^2\rangle}{M\langle \mu^2\rangle} \tag{5}$$

The electron-phonon coupling constant (λ) can be estimated using the electronic bandstructure results by using the relation (5). Where I^2 is the electron-phonon interaction matrix element averaged over the Fermi surface [16], M is the molecular mass, and $\langle \mu^2 \rangle$ is the average phonon frequency square (6) given by [17]

$$\langle \mu^2 \rangle = \frac{1}{2}\Theta_D^2 \tag{6}$$

and

$$\langle I^2 \rangle = 2\sum_l \frac{(l+1)}{(2l+1)(2l+3)} M^2_{l,l+1} \frac{N_l(E_F) N_{l+1}(E_F)}{N(E_F) N(E_F)} \tag{7}$$

with Θ_D in energy units. The quantity $\langle I^2 \rangle$ is determined by the relation (7). Where $M_{l,l+1}$ is the electron-phonon matrix element which can be expressed in terms of the logarithmic derivate (D_l)

$$M_{l,l+1} = -¤_l ¤_{l+1}\left[(D_l(E_F) - l)(D_{l+1}(E_F) + l + 2) + (E_F - V(S))S^2\right] \tag{8}$$

where $V(S)$ is the one electron potential and $¤_l$ is the sphere boundary amplitude of the *l* partial wave function evaluated at E_F. The parameter N_1 in (7) is the partial density of states function for the angular momentum quantum number *l*. The superconducting transition temperature (T_C) which is obtained by using the procedure detailed below.

The superconducting transition temperature is calculated using Allen-Dynes formula [18] which is given by

$$T_C = \frac{\langle \mu \rangle}{1.45} \exp\left[\frac{-1.04(1+ª)}{ª - «^*(1+0.62ª)}\right] \tag{9}$$

where λ is the electron-phonon coupling constant which can be estimated as detailed above, and μ* is the electron-electron interaction constant. The μ* can be obtained from the empirical relation given by Bennemann and Garland [19, 20],

$$\lambda^{*} = \frac{0.26\, N(E_F)}{1 + N(E_F)} \tag{10}$$

TABLE 3 ELECTRON-PHONON INTERACTION CONSTANT (Λ) AND SUPERCONDUCTING TRANSITION TEMPERATURE (T_C) FOR V_3AU

Compound	**λ**		**T_C (K)**	
	Present	*Expt.*	*Present*	*Expt.*
V_3Au	0.69	0.50 [7] 0.69 [15] 0.54 [21]	2.76	2.00 [7] 2.87 [15] 2.97 [21]

The calculated and experimental values of λ and T_C are presented in Table 3. The values estimated by the present work for V_3Au agrees well with the experimental values that are reported previously [7, 15 & 21].

V. CONCLUSIONS

The electronic band structure studies of vanadium based A15 superconductor V_3Au is carried out, by using the TB-LMTO method. The ground state properties such as equilibrium lattice parameters and primitive cell volume have been obtained by fitting the electronic total energy with the Murnaghan equation of state and are in good agreement with the experimental results. The electronic band structures show a strong hybridization between *p*- and *d*-bands and are also narrowly piled up around the Fermi energy for the material and it is also evident in the density of states results. Furthermore, it is found that the band structure and related properties at the Fermi energy are dominated by the *d*-bands originating mainly from vanadium alloy. The density of states at the Fermi energy is found to be strongly influenced by the *d*-bands of atoms due to V_3Au. The calculated values of $\Theta_{D,}$ γ, λ and T_C are observed to be in good agreement with the available experimental results existing in the literature. Thus the present studies have provided a better understanding of the fundamental electronic and superconducting properties of V_3Au superconducting compound.

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