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Study of Total energy, equation of state and energy volume relation for Al, Ni and it binary alloys

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Abstract *– In the present paper our well establish local model potential describing electron ion interaction is used to study atomic properties of Al, Ni metals and its binary alloys (NiAl, Ni_3Al) along with three different local field correction functions due to Hartree (H), Ichimaru and Utsumi (IU) and Sarkar et al (S). Here the parameter of potential is determined using the equilibrium condition at zero pressure. The total energy and equation of state of the metals are computed using higher order perturbation theory based on pseudopotential formalism. Numerical values of total energy obtained for metals are found superior than the other theoretical findings. Good agreement is achieved between the presently calculated results of equation of state with experimental and available other data found in the literature, confirming the applicability of our model potential for such study.*

Keywords*: Total energy, equation of state, pseudopotential.*

I. Introduction

Recently Vyas et al [1] and Bariya et [2] have reported the total energy and equation of state for the alkaline earth metal and some transition metals using the pseudopotential approach. This work has motivated us to calculate total crystal energy, equation of state and energy-volume for Al, Ni and NiAl and Ni_3Al binary system using the pseudopotential theory and second order perturbation theory. We have selected these alloys, because of their extraordinary properties and many applications in the industry [2]-[6].

The atomic properties like total crystal energy, pressure, energy – volume relations and pressure – volume relations are computed for Al, Ni (FCC) and NiAl, Ni_3Al(FCC) using the reciprocal sum analysis method. The well tested model potentials [7] along with three different forms of local field correction functions (LFCF) namely Hartree [7], Ichimaru-Utsumi [7], Sarkar Sen et al [7] local field correction functions to compute the screened form factors, which are then used to calculate the total energy and equation of state for many solid solutions of interest.

II. Theory and method of computation

The first work on the band energy of alloy was done by Hayes and co-workers [8] using a non-local potentials. Gajjar et al [9] have reported the total binding energy for all the alkali metals and its binary system using a model potential which is continuous in r-space. Soma [10], [11] was successful in computing total energy and bulk modulus of some co-valent compounds on the basis of extended perturbation theory. They have used historical model potentials and local Heine-Abarenkov model potential [12] with an additional parameter to ensure minimum energy condition.
The total crystal energy per pseudo-atom, E(x), of the binary alloy can be obtained in the framework of the usual second order perturbation as [9],[10]

$$E(x) = E_i(x) + E_{es}(x) + E_1(x) + E_2(x) \quad (1)$$

In equation (2), E_i is the electrostatic energy of point ions immersed in the uniform gas of valence electrons, called the Madelung energy, which is given by

$$E_i(x) = -\frac{\alpha Z^2}{R_a} \quad (2)$$

Here α is the Madelung's constant and $R_a = r_s Z^{\frac{1}{3}}$, Here r_s is the radius of the sphere containing one electron. In Equation (1),E_{es} is the sum of the kinetic, exchange and correlation energies of the valence electron and is given by

$$E_{es}(x) = Z\left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} - 0.115 + 0.031\ln(r_s)\right] \quad (3)$$

E_1 is the First order perturbation energy of the valence electron due to the pseudopotential and is given by,

$$E_1(x) = \lim_{q\to 0}\left[\frac{4\pi Z^2 e^2}{\Omega_0 q^2} + ZW_B(q)\right] \quad (4)$$

and

$$E_2(x) = \sum_{q\neq 0} F(q) \quad (5)$$

is the band structure energy. Here F(q) is the normalized energy wave number characteristics and is given by

$$F(q) = -\frac{\Omega_0 q^2}{16\pi}\left|V_B(q)\right|^2 \times \frac{\left[\varepsilon_H(q) - 1\right]}{\left\{1 + \left[\varepsilon_H(q) - 1\right]\left[1 - f(q)\right]\right\}} \quad (6)$$

Where $V_B(q)$ is the bare ion pseudopotential from factor is given by [7].

$$V_B(q) = -\frac{4\pi^2 e^2}{\Omega_0 q^2}\left(\cos(qr_c) - \frac{\exp(-1)\ qr_c}{1+(qr_c)^2}(\sin(qr_c) + qr_c\cos(qr_c))\right) \quad (7)$$

The pseudopotential form factor used to describe the electron-ion interaction in metals of the form (in Rydberg Units). Where Z, Ω_0, q and r_c are valency, atomic volume, wave vector and parameter of the potential respectively. The potential of this type is representative of self consistent potentials with single parameter r_c.

The pressure P is obtained from the first derivative of the total crystal energy per atom E with respect to the atomic volume Ω_0 given by,

$$P_T = -\frac{dE_T}{d\Omega_0} \quad (8)$$

$$\therefore P_{tot} = -\left[\frac{dE_i}{d\Omega_0} + \frac{dE_{es}}{d\Omega_0} + \frac{dE_1}{d\Omega_0} + \frac{dE_2}{d\Omega_0}\right] \quad (9)$$

We can write the above equation as

$$P = P_i + P_0 + P_1 + P_2 \quad (10)$$

By setting the derivative

$$\frac{dE}{d\Omega_0} = -P = 0 \quad (11)$$

The total crystal energy at zero pressure for Al, Ni and its binary alloys is found using Equation (1) to Equation (8).

III. Results and Discussions

TABLE I – IN PUT PARAMETER AND CONSTANTS

Metals	Z	Ω_0 (a.u)^3	r_c (a.u)		
			H	IU	S
Al	3	111.3	0.6303	0.6131	0.6258
Ni	1	73.793	0.5531	0.5512	0.5517
NiAl	2	92.547	0.5853	0.5723	0.5819
Ni_3Al	1.5	83.17	0.5655	0.5579	0.5628

III.1. Total energy

TABLE II- VARIOUS CONTRIBUTIONS TO THE TOTAL ENERGY AT ZERO PRESSURE

Metals/ alloys	Various contribution of energy (Ryd)				
	LFCF	E_i	E_0	E_1	E_2
Al	H	-5.4040	-0.0567	0.9977	-0.2438
	IU	-5.4040	-0.0567	0.9441	-0.2553
	S	-5.4040	-0.0567	0.9837	-0.2046
Ni	H	-1.5493	-0.0972	0.2621	-0.0450
	IU	-1.5493	-0.0972	0.2562	-0.0466
	S	-1.5493	-0.0972	0.2607	-0.0402
NiAl	H	-2.5541	-0.1118	0.4598	-0.0898
	IU	-2.5541	-0.1118	0.4396	-0.0981
	S	-2.5541	-0.1118	0.4546	-0.0769
Ni_3Al	H	-1.4887	-1.2089	0.2687	-0.0398
	IU	-1.4887	-1.2089	0.2615	-0.0415
	S	-1.4887	-1.2089	0.2661	-0.0356

TABLE III- TOTAL ENERGY AT ZERO PRESSURE FOR ALUMINUM (Al)

LFCF	Total energy (Ryd)	% error	Exp. [13]	Others [14-15]
H	-4.7068	11.9	-4.142	-4.343 -4.392
IU	-4.7720	13.1		-4.279
S	-4.6816	11.5		-4.192 -4.327

TABLE IV- TOTAL ENERGY AT ZERO PRESSURE FOR NICKEL (Ni)

LFCF	Total energy (Ryd)	% error	Exp. [2]	Others [2]
H	-1.4295	4.77	-1.3612	-1.373, -1.214, -1.074
IU	-1.4368	5.26		
S	-1.4261	4.55		

TABLE V- TOTAL ENERGY AT ZERO PRESSURE FOR $NiAl$ AND Ni_3Al BINARY ALLOYS

LFCF	Total energy (Ryd) NiAl	Total energy (Ryd) Ni_3Al	Exp.	Others
H	-2.2959	-1.3808	---	---
IU	-2.3244	-1.3933		
S	-2.2909	-1.3791		

The input and constant used in the present work are shown in the Table I. Table II shows the various contribution of total energy. From Table III and IV we can see that the total crystal energy for the pure Aluminum and pure Nickel along with the experimental [13], [2] and other available values [14], [15] respectively. The total crystal energy as calculated using model potential along with S function shows good agreement with experimental and other available data then the other screening functions. It is observed that S screening functions shows 11.5 % to 4.55% and IU screening functions show deviation 13.1% to 5.26% from experimental data in comparison to the other screening functions for Al and Ni respectively. Here we are reporting for the first time the total crystal energy for the two different binary alloys NiAl and Ni3Al using local model potential. Table IV shows the total energy at zero pressure for NiAl and Ni_3Al binary alloys. From Table IV it is observed that the maximum total energy obtained due to IU functions while minimum total energy obtained due to S functions. However, in the absence of any such experimental finding and other data, we do not put any remark for these alloys at this stage but present results might serve a useful set of results for further research in this field.

III.2. Pressure and Volume(P-V) relation

The behavior of various materials under compression finds application in the field of materials science and technology. In the present study we have calculated the Pressure-Volume relation for the Al, Ni and its binary alloys. These solid binary alloys have contained properties like light weight, high strength and hardness, low mass etc and these alloys are particularly attractive for transport application such as automobiles and weight reduction for industrial instruments. The emerging concept of system materials design provides such opportunities.

The P-V relation for Al has been shown in Fig 1. it has been observed that the P-V relation calculated with H screening function shows minimum deviation compared to other two local field correction functions and it is observed that present computed results is good agreement with the experimental data [5] and Hungoniot data [16].Thus, model potential along with three local field correction functions, the H function gives better results for P-V relation for pure Al.

Out comes of the present results for EOS in Fig. 2 are not found in good agreement with the experimental [17] and other data [2] for Ni, because they have taken the valency higher than that employed in the present approach.

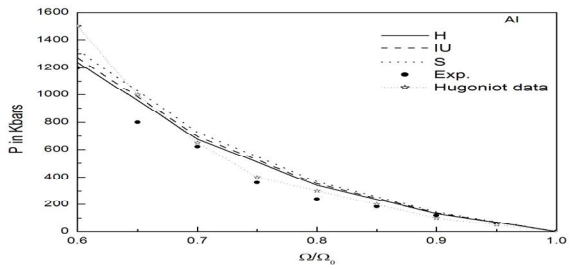

Fig. 1. Pressure-Volume relation for Al along with Exp. [16] and Hugoniot data [16]

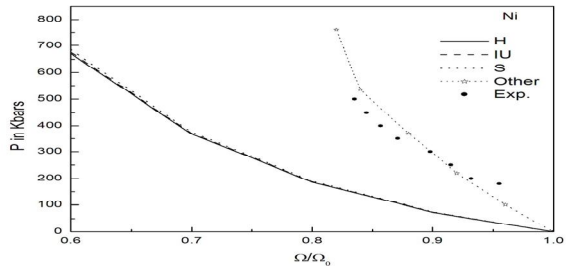

Fig. 2. Pressure-Volume relation for Ni along with Exp.[17] and other data [2]

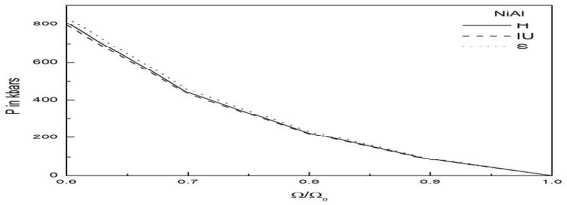

Fig. 3. Pressure-Volume relation for NiAl.

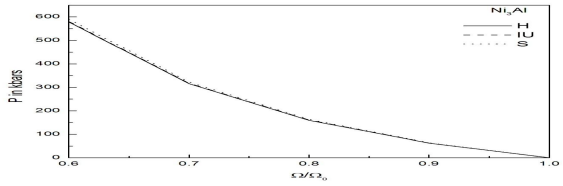

Fig. 4. Pressure-Volume relation for Ni_3Al.

Here, as a case study for the first time we have reported theoretical calculation for the pressure- volume relation for NiAl and Ni_3Al binary systems using local model potential and results are as shown in fig. 3 and 4 respectively. In all binary systems it has been observed that all screening functions show the same trend. Under the 200 kbars pressure all screening functions overlap each other and at higher pressure S function s shows the some significant influence with respect to H screening functions.

III.3. Energy and Volume(E-V) relation

From the fig.5 to 8 we can infer that all the local filed correction functions show the similar trend. It is seen that IU screening function shows the maximum and S screening functions shows minimum influence with respect to H screening function.

Fig. 7 shows the energy-volume relation for the NiAl binary system. For the energy-volume relation the computed percentile influence with respect to H function are 1.04%-1.28% when IU is employed and 0.28%-0.18% when S screening functions is employed. Fig 8 shows the energy –volume relation for Ni_3Al binary system. For the energy-volume relation the computed maximum and minimum percentile change with respect to H function are found to be 2.12%-2.15% and 0.15%-0.72% in the case of IU, and S screening functions respectively. The direct experimental and other data for E-V relation are not available; the results may be used for correlating other properties of this binary system.

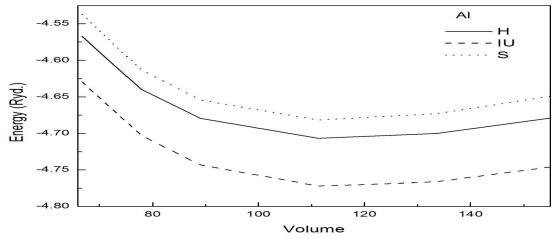

Fig. 5. Energy-Volume relation for Al.

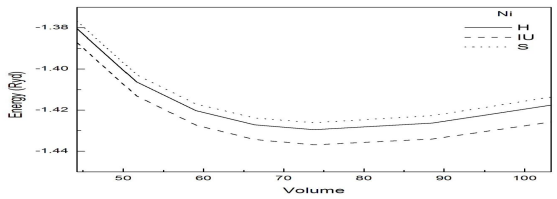

Fig. 6. Energy-Volume relation for Ni.

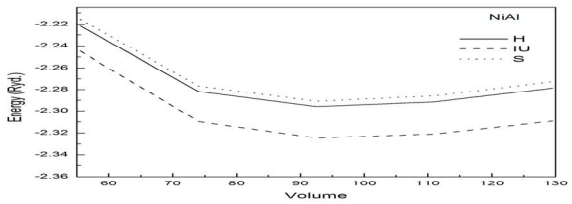

Fig. 7. Energy -Volume relation for NiAl.

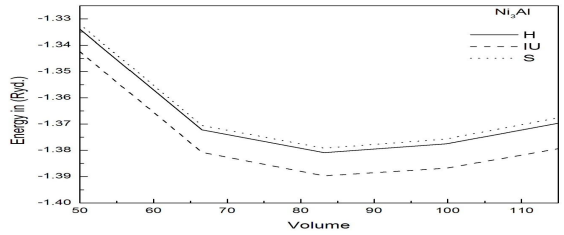

Fig. 8. Energy –Volume relation for Ni_3Al.

IV. Conclusion

Lastly we conclude that the total crystal energy computed using the S screening functions found to be better achieving with experimental data and other available data. Pressure –volume relation found for the Al metal shows good agreement with experimental data and other available data. For Ni the equation of state does not show good agreement with experimental and available data because in the transition metals valency play vital role for calculated equation of state. Present study is going to provide the important information regarding the P-V and E-V relation for binary system of NiAl and Ni_3Al.

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