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Second Order Elastic Constants of Nickel, Gold and Silver

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Abstract: second order elastic constants of Ni, Au and Ag are carried out by taking simple two body potential $\Phi = - A r^{-n} + B \exp(-Pr^{m})$. Potential parameters are calculated by taking experimental values of lattice constant, bulk modulus and cohesive energy. Computed results of second orders elastic constants are close with experimental results.

Keywords: Two body potential, Bulk modulus, Energy per unit cell, Elastic constant, Cohesive energy and Lattice constant.

1. INRODUCTION

Second order elastic constants (SOEC) play an important role in solid state physics. Many workers [1-21] calculated second and third order elastic constants (TOEC) by taking different types of interaction between atoms. Lincon et al [1], Girifalco et al [2], and Singh et al [3-5] have estimated SOEC and TOEC of many cubic metals using Morse and generalized Morse potential as an interaction between atoms. Temperature dependency of elastic constants was study by Telichko et al [6] and Singh [7]. Golesorkhtabar et al [8] and Dai et al [9] have evaluated elastic constants of some cubic metals and alloy. Verma et al [10] have calculated cohesive energy, SOES and phonon spectra of fcc Platinum using extended generalized exponential potential. Using the same potential Verma et al [11] calculated SOEC and TOEC for many cubic metals. Ciftci et al [16] investigated effect of pressure on mechanical properties such as elastic constants and bulk modulus of many cubic metals. They used modified many body Morse potential function in the framework of M D simulation. They also calculated PV calculations for same metals. Fae'q et al [18] have calculated elastic constants of Cu, Ag and its alloys. Using ab initio and semi empirical approach Kociskova et al [19] evaluated SOEC of Al, Cu and Ni. Wang et al [20] have calculated second, third and fourth order elastic constants of Cu, Al, Au and Ag using ab initio density function theory. Recently Pishkenari et al [21] estimated SOEC of eight cubic metals included Ni, Au and Ag using EAM approach. These studies show that calculation of SOEC of cubic metals is active field in present time.

To calculate SOEC of Ni, Au and Ag, we have used simple two body potential which is proposed by Kuchhal et al [12] and recently used by Singh [22] for calculation of SOEC of Cu and Al. This potential has two adjustable parameters and three unknown parameters which are calculated by taking experimental values of lattice constant, bulk modulus and cohesive energy. Thus the purpose of present work is to develop a new potential and calculate SOEC as an application of this potential for Ni, Au and Ag.

2. TWO BODY POTENTIAL

Two body potential as suggested by Kuchhal and Das [12] is given by

$$\phi = -Ar^{-n} + B\, exp(-Pr^{m})$$

Where A, B and p are positive constant and are expressed in unit of erg.cm^{n}, erg and cm^{-m} respectively and r gives the distance from the lattice site with coordinate specified by the three integers l_1, l_2, l_3 .

$$\mathrm{r} = \frac{1}{2}\left(a_1^2 l_1^2 + a_2^2 l_2^2 + a_3^2 l_3^2\right)^{\frac{1}{2}}$$

Where l_1, l_2 and l_3 are integers (chosen such that $l_1 + l_2 + l_3$ is even for an fcc lattice) and a_1, a_2 and a_3 are cell lengths. Since this potential is empirical in nature, there is no limit to the number of different functions, which can be calculated from a given set of experimental data. Thus any family of potential function should include relatively short-range steep potential as well as longer range shallower potentials. This potential contains two adjustable parameters m, n and three unknown potential parameters A, B and P which can be calculated by using experimental values of lattice constant, bulk modulus and cohesive energy as an input data.

Following Girifalko et al [2], and Singh et al [3-5] recently Singh [22] developed a method for evaluation of unknown potential parameters A, B and P by taking experimental values of lattice constant, bulk modulus and cohesive energy as an input data. We take same method for evaluation of potential parameters of K D potential. The detailed method and mathematical expressions for calculation of potential parameters are given in reference [22], so here we have discussed the result only. Table 1 gives the input data [23] i.e. the experimental value of lattice constant, bulk modulus and cohesive energy for Ni, Au and Ag.

Metals	Lattice constant (Å)	Cohesive energy (10^{-12}erg)	Bulk modulus (10^{12}dyn/cm^2)
Nickel	3.5238	7.1128	1.86
Gold	4.0783	6.1036	1.732
Silver	4.0856	4.7259	1.007

Table: - 1 Input data for Ni, Au and Ag [23].

3. SECOND ORDER ELASTIC CONSTANTS OF CUBIC METAL

Expressions for second order elastic constants C_{11} and C_{12} are present in literature (see in reference [12]).

$$c_{11} = \frac{u\,a_0}{8} \sum_{l_1} \sum_{l_2} \sum_{l_3} l_1^4 \frac{d^2\emptyset}{(dr^2)^2}$$

$$c_{12} = \frac{u\,a_0}{8} \sum_{l_1} \sum_{l_2} \sum_{l_3} l_1^2 l_2^2 \frac{d^2\emptyset}{(dr^2)^2}$$

Where u gives number of atoms per unit cell which is four for fcc metals. Using simple mathematics we can find out second derivative of potential function with respect to r^2 and with the help of these equations we can calculate SOEC.

4. RESULTS AND DISCUSSION

Table 2 gives the calculated potential parameters for Ni, Au and Ag. Figures from 1 to figure 3 show the variation of energy per unit cell (E) with respect to lattice constant a (Å) ($a = a_1 = a_2 = a_3$) for Ni at different fixed values of adjustable parameters m and n. Similarly figures from 4 to figure 6 show the variation of energy per unit cell with respect to lattice constant a (Å) for Au at different fixed values of adjustable parameters m and n and figures from 6 to figure 9 show the variation of energy per unit cell with respect to lattice constant a (Å) for Ag at different fixed values of adjustable parameters m and n. These figures show that at different values of adjustable parameters we can find out short range steep potentials as well as longer range shallower potentials.

Metals	Adjustable parameters		Unknown parameters		
	m	n	P (cm^{-m})	A (erg. cm^n)	B (erg)
Nickel (Ni)	1	1/5	5.2063×10^{9}	1.3562×10^{-16}	3.9962×10^{41}
	1	½	2.107×10^{9}	1.2514×10^{-18}	7.201×10^{8}
	1	2	5.628×10^{8}	6.8755×10^{-29}	2.4217×10^{-7}
	2	1/5	1.0528×10^{17}	1.3562×10^{-16}	4.4302×10^{13}
	2	1	2.2405×10^{16}	4.9729×10^{-22}	4.8596×10^{-8}
Gold (Au)	1	1/5	7.55×10^{9}	1.1975×10^{-16}	3.3755×10^{79}
	1	½	3.04×10^{9}	1.1508×10^{-18}	6.9101×10^{23}
	1	2	7.89×10^{8}	7.4295×10^{-29}	7.463×10^{-4}
	2	1/5	1.314×10^{17}	1.1975×10^{-16}	2.674×10^{32}
	2	1	2.728×10^{16}	4.8686×10^{-22}	1.6332×10^{-4}
Silver (Ag)	1	1/5	5.694×10^{9}	9.2784×10^{-17}	2.642×10^{56}
	1	½	2.298×10^{9}	8.9351×10^{-19}	4.06×10^{14}
	1	2	6.05×10^{8}	5.946×10^{-29}	3.9636×10^{-6}
	2	1/5	9.92×10^{16}	9.2781×10^{-17}	8.6176×10^{20}
	2	1	2.083×10^{16}	3.8026×10^{-22}	8.2785×10^{-7}

Table: - 2 Potential parameters of Ni, Au and Ag for different values of adjustable parameters m and n.

We see from these figures that adjustable parameters m and n change breadth of potential. Breadth of the potential is highly change by adjustable parameter n, and very small change occur by adjustable parameter m. From these results we conclude that by decreasing the adjustable parameter n we found long range potential (i.e. breadth of potential increase) and by increasing the adjustable parameter n we found short range potential (i.e. breadth of potential decrease). The depth of the potential is not depends on adjustable parameters m and n.

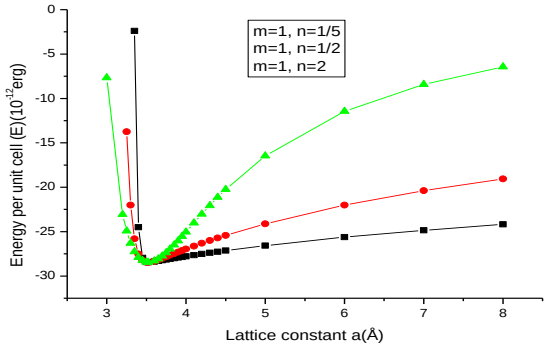

Figure :- 1 Variation of energy per unit cell with respect to lattice constant a (Å) of Ni for different adjustable parameters m and n.

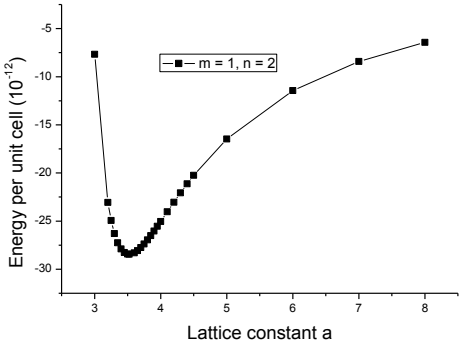

Figure :- 2 Variation of energy per unit cell with respect to lattice constant a (Å) of Ni for adjustable parameters m =1 and n = 2.

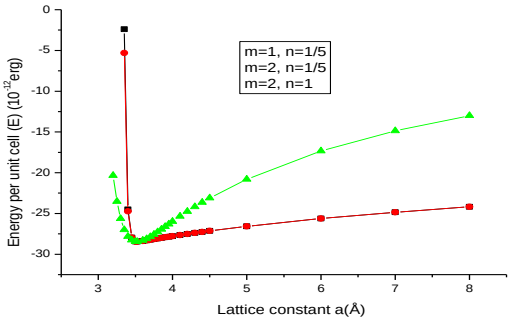

Figure: - 3 Variation of energy per unit cell with respect to lattice constant a (Å) of Ni for different adjustable parameters m and n.

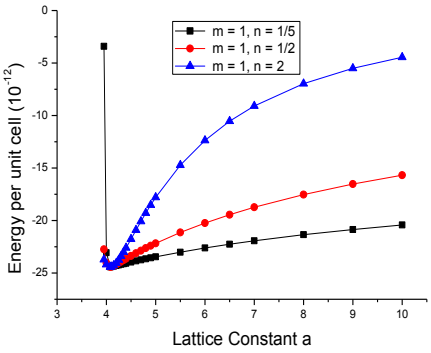

Figure: - 4 Variation of energy per unit cell with respect to lattice constant a (Å) of Au for different adjustable parameters m and n.

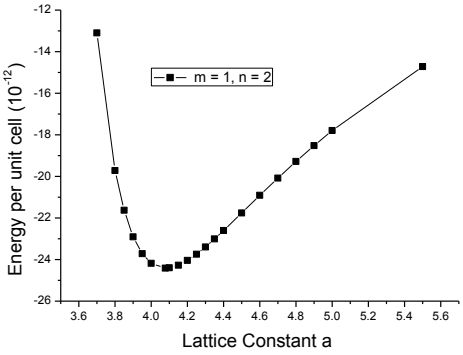

Figure: - 5 Variation of energy per unit cell with respect to lattice constant a (Å) of Au for adjustable parameters m =1 and n = 2.

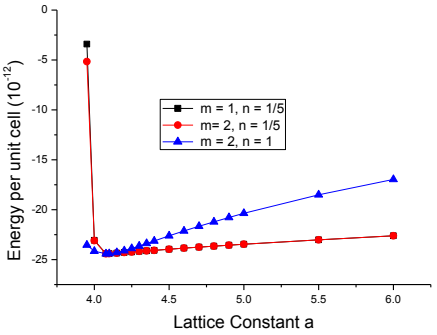

Figure: - 6 Variation of energy per unit cell with respect to lattice constant a (Å) of Au for different adjustable parameters m and n.

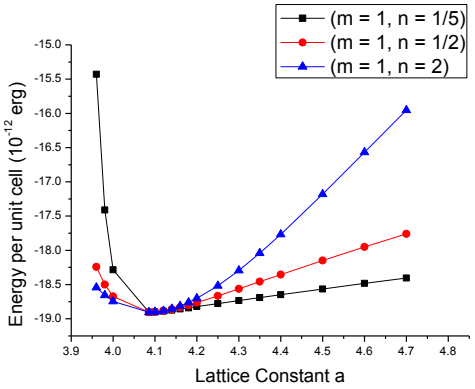

Figure: - 7 Variation of energy per unit cell with respect to lattice constant a (Å) of Ag for different adjustable parameters m and n.

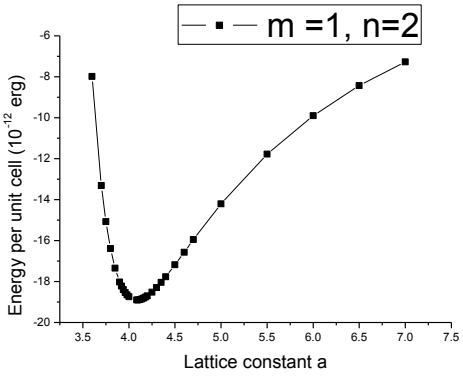

Figure: - 8 Variation of energy per unit cell with respect to lattice constant a (Å) of Ag for adjustable parameters m = 1 and n =2.

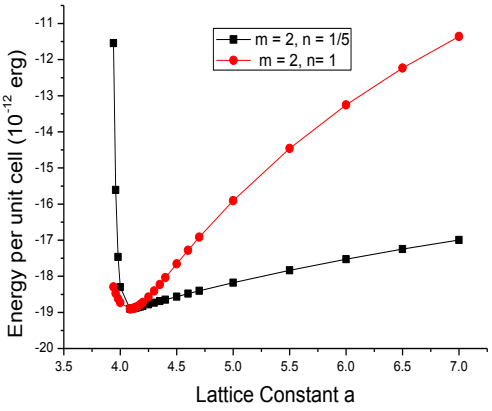

Figure: - 9 Variation of energy per unit cell with respect to lattice constant a (Å) of Ag for different adjustable parameters m and n.

Adjustable parameters		Second order elastic constants (x 10^{12} dyn / cm^2)	
m	n	C_{11}	C_{12}
1	1/5	2.7858	1.3971
1	1 /2	2.7765	1.4018
1	2	2.6509	1.4643
2	1/5	2.7858	1.3971
2	1	2.7504	1.415
Experimental results [23]		2.612	1.508
Other study [24]		2.3806	1.6883
Other study [21]		2.64	1.57

Table: - 3 SOEC of Ni for different values of adjustable parameters m and n.

Adjustable parameters		Second order elastic constants (x 10^{12} dyn / cm^2)	
m	n	C_{11}	C_{12}
1	1/5	2.5978	1.3013
1	1 /2	2.5918	1.3034
1	2	2.5205	1.3381
2	1/5	2.5957	1.3002
2	1	2.5774	1.3104
Experimental results [23]		2.016	1.697
Other study [24]		2.3403	1.4963
Other study [21]		1.83	1.59
Other study [16]		1.954	1.637
Other study [17]		1.5	1.286

Table: - 4 SOEC of Au for different values of adjustable parameters m and n.

Adjustable parameters		Second order elastic constants (x 10^{12} dyn / cm^2)	
m	n	C_{11}	C_{12}
1	1/5	1.5089	.75623
1	1 /2	1.5045	.75802
1	2	1.4505	.78584
2	1/5	1.5097	.75662
2	1	1.4943	.764
Experimental results [23]		1.315	.973
Other study [24]		1.2546	.8584
Other study [21]		1.24	.94
Other study [16]		1.326	.984
Other study [17]		.832	.791

Table:- 5 SOEC of Ag for different values of adjustable parameters m and n.

Tables from 3 to 5 give calculated values of second order elastic constants of Ni, Au and Ag at different values of adjustable parameters m and n. Pishkenari et al [21] and Pamuk et al [24] have calculated SOEC of Ni using very tedious mathematics for interaction between atoms and the results of these study are not too much differ from our results. Similarly Pishkenari et al [21], Ciftci et al [16], Pandya et al [17] and Pamuk et al [24] have calculated SOEC of Au and Ag by using ab initio, M D simulation and EAM approach for interaction between atoms which also have too complicated mathematics. Our calculated results of SOEC are close to experimental results in comparison to other study and the potential which is used in present work have very simple mathematics.

5. CONCLUSION

Potential used in this work is very simple since it has only two adjustable parameters and three unknown parameters. Potential parameters are calculated by using only three experimental physical quantities. We also show the breadth of potential is depends on adjustable parameter n. Our calculated results of SOEC for all three cubic metals are close to experimental results.

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