Pressure Volume Calculations in FCC Metals using Two Body Potentials

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Pressure volume (P-V) calculations of FCC metals (Copper, Silver, Gold, Aluminum and Nickel) have been carried out by taking simple two body Kuchhal and Das (K. D.) and Morse potential. In case of K. D. potential, the computed results of P-V calculations are fairly close with experimental results. At high relative volume, the computed results with Morse potential are closely match with experimental results but at low relative volume, calculated and experimental results are poor match. Our study shows that computed results with K. D. potential gives better results of P-V calculations for all FCC metals in comparison to computed results with Morse potential.

Keywords: Two body potential, FCC metals, Mechanical properties, Elastic constants.

1. INTRODUCTION

Due to geophysical and technological applications of pressure volume (P-V) calculations, theoretical and experimental work on this problem is quite interesting in recent year. Many investigators [1-6] estimated P-V calculation of cubic metals using different type of interaction between atoms. Milstein [1] calculated P-V calculations of 8 cubic metals including Cu, Ag, Au, Al and Ni by taking Morse potential as an interaction between atoms. Using logarithmic potential, Thakur [2] investigated P-V calculations of FCC metals (Nickel and Thorium) and BCC metals (V, Mo and W-α). Using embedded atom model (EAM), Chantasiriwan & Milstein [3,4] and Ciftci & Colankoglu [5] also carried out P-V calculation of some cubic metals. Using modified many body Morse potential in the frame work of M D simulation, Ciftci *et. al.* [6] investigated P-V calculations of many cubic metals. Matthew *et. al.* [7] measured high pressure and temperature equation of state of Cobalt anvil cell in conjunction with synchrotron X- ray diffraction. Using F. S. potential, Dai *et. al.* [8] estimated P-V calculations and many other mechanical properties of cubic metals such as Cu, Ag, Au, Pd and Pt. Shim *et. al.* [9] are reported PVT equation of state of Gold based on the inversion of quasi-hydrostatic compression and shock wave data. Two and three body potential energy and equation of state of solid Argon are recently accurately calculated by Zheng [10] in the higher experimental studied range of pressure (0-80 GPa). For Gold and Aluminum, Dewaele *et. al.* [11] have measured compression verses pressure at ambient temperature. These studies showed that, in the present time the theoretical research work on P-V calculations of cubic metals is an active field.

Recently Singh and coworkers calculated second order elastic constants [12,13], third order elastic constants, pressure derivatives of second order elastic constants [14,15] and theoretical strength [16] of many FCC metals using two body potential which is proposed by Kuchhal and Dass (K. D.) [17]. Computed results of these mechanical properties of FCC metals are close agreement with experimental results in comparison to other two body potentials. Thus these studied showed that the K. D. potential gives better results of mechanical properties of FCC metals in comparison to other two body potentials. This gives us a motivation to estimate P-V calculations of FCC metals using K. D. potential. First section of this study gives introduction and present situation of work, second section gives details of two body potentials, third section gives mathematical equation of P-V calculations, fourth section gives results and discussion of the work, fifth section gives the conclusion of the present work and the last section gives references of the present study.

2. TWO BODY POTENTIAL

Two body potential as suggested by Kuchhal and Dass [17] is given as

$$\phi(r) = -Ar^{-n} + Bexp(-pr^{m})$$

Where A, B and p are positive constants and are expressed in unit of erg.cm^{n}, erg and cm^{-m} respectively. The potential parameters A, B and p are determined by using the experimental values of lattice constant, bulk modulus and cohesive energy keeping m and n as an adjustable parameters. Singh and coworker [12,13] developed a method for evaluation of potential parameters of K. D. potential and are given in Table 1.

Table 1: Potential parameters of K. D. potential [12,13] and Morse potential [1,18,19].

Elements		Cu	Ag	Au	Al	Ni
Lattice parameter (Å) [20]		3.6153	4.0856	4.0783	4.049	3.5238
K. D. potential [12,13]	m	1	1	1	1	1
	n	4	4	7	4	4
	p(10^{8} cm^{-1})	3.2318	3.3838	3.3452	2.4198	3.288
	A(erg-cm^{n})	3.9266 x10^{-43}	4.7565 x10^{-43}	5.451 x10^{-65}	7.1788 x10^{-43}	4.5426 x10^{-43}
	B(10^{-9} erg)	3.251	9.427	40.426	1.1502	3.917
Morse potential [1]	α (Å^{-1})	1.3392	1.0239	.4766	2.7116	2.4876
	r_0(Å)	2.885	3.4588	5.9845	2.8776	2.5275
	D(10^{-12}erg)	.5677	.6856	1.4449	.1544	.3506
Morse potential [19]	α (Å^{-1})	1.3588	1.369	-	1.1646	1.4199
	r_0(Å)	2.866	3.115	-	3.253	3.253
	D(10^{-12}erg)	.5494	.5324	-	.433	.433
Morse potential [18]	α (Å^{-1})	1.3921	1.3939	1.6166	-	1.3921
	r_0(Å)	2.838	3.096	3.004	-	2.838
	D(10^{-12}erg)	.55212	.5278	.7732	-	.6856

Morse potential function is given as

$$\phi(r) = D(e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)})$$

D, α and r_0 are three unknown potential parameters which are determined by many workers for different cubic metals using some physical quantities as an input data. Morse potential parameters of many cubic metals are estimated by Flahive *et. al*. [18], Girifalco [19] and Milstein [1]. These potential parameters are shown in Table 1 for Cu, Ag, Au, Al and Ni. In all these equations r gives the distance from a lattice site chosen as the origin to a given lattice site with coordinate specified by the three integers l_1, l_2, l_3 as

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

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. In equilibrium, $a_1 = a_2 = a_3 = a_0$, where a_0 is equilibrium lattice parameter and is show in Table 1.

3. PRESSURE VOLUME CALCULATIONS

For hydrostatic pressure, the all lattice parameters a_i are equal i.e. ($a_1 = a_2 = a_3 = a$) and the pressure P (at T = 0K) is given [1] by

$$P = \frac{u}{4a} \sum_{l_1} \sum_{l_2} \sum_{l_3} l_1^2 \frac{d\emptyset}{dr^2}$$

And the corresponding relative volume is given by

$$\frac{V}{V_0} = \left(\frac{a}{a_0}\right)^3$$

Here u gives the number of atoms per unit cell, which is four for FCC metals. Using simple mathematics we can find out first derivative of potential function with respect to r^2 and we can calculate pressure with the help of this equation.

4. RESULTS AND DISCUSSION

Calculated values of pressure P at different values of relative volume (V/V_0) are shown in Table 2, 3 and 4. These tables give the computed results of P-V calculations using three Morse potential and K. D. potential. Computed results are also compared with experimental results of McQueen *et. al.* [21]. As per our knowledge, the experimental results of Aluminum are not available in literature so they are not shown in Table 3.

Table 2:- Pressure volume calculations of Cu and Ag.

Copper					
	Pressure P (Kbar)				
V/V_0	Exp. [21]	K. D.	Morse Milstein [1]	Morse Girifalco [19]	Morse Flahive [18]
.99	0	14.1	14.5	3.74	-7.4
.933	100	113	115.4	99.9	88.3
.89	200	213.5	216.0	196.2	184.5
.856	300	313.6	314.8	290.3	279.7
.827	400	416.8	415.6	387.8	377.3
.803	500	517.3	512.8	481.4	471.7
.782	600	618.3	609.7	574.8	566.2
.764	700	716.0	702.8	664.6	657.2
.748	800	812.8	794.4	735.1	746.9
.734	900	905.9	882.1	837.9	833.0
.72	1000	1007.7	977.6	930.2	926.9
.708	1100	1102.6	1066.1	1015.9	1014.1
.696	1200	1205.3	1161.5	1108.3	1108.3
.686	1300	1293.3	1246.6	1190.8	1192.4

Silver					
	Pressure P (Kbar)				
V/V_0	Exp. [21]	K. D.	Morse Milstein [1]	Morse Girifalco [19]	Morse Flahive [18]
.987	0	13.7	14.7	3.45	-3.45
.918	100	109.5	111.4	95.9	87.41
.872	200	202.1	198.4	183.1	173.6
.836	300	297.0	283.0	270.6	260.4
.806	400	395.2	367.3	360.1	349.4
.781	500	493.7	448.9	448.5	437.5
.760	600	590.3	.526	534.4	523.2
.742	700	685.0	601.3	617.7	606.4
.725	800	785.8	679.1	705.7	694.6
.711	900	878.4	749.1	785.9	774.9
.698	1000	973.0	819.5	867.3	856.5
.686	1100	1068.4	889.4	948.9	938.3
.674	1200	1172.2	964.5	1037.2	1027.1
.664	1300	1266.2	1031.4	1116.5	1106.8

Table 3: Pressure volume calculations of Au and Al.

Gold					Aluminum			
	Pressure P (Kbar)					Pressure P (Kbar)		
V/V_0	Exp. [21]	K. D.	Morse Milstein [1]	Morse Flahive [18]	V/V_0	K. D.	Morse Milstein [1]	Morse Girifalco [19]
.989	0	19.7	72.9	-2.1	.95	41.5	51.0	31.9
.943	100	119.0	182.7	96.28	.9	95.86	132.4	86.9
.907	200	219.2	285.6	197.7	.85	167.3	261.1	159.8
.878	300	317.7	381.6	299.1	.8	261.6	463.9	256.7
.852	400	422.2	479.4	408.5	.75	386.6	784.5	386.4
.831	500	519.5	567.7	511.9	.7	553.7	1295.6	561.1
.812	600	618.9	655.6	618.9	.65	779.4	2120	799.2
.795	700	718.1	741.6	727.0	.6	1087.8	3474.5	1127.7
.778	800	828.0	835.2	848.4	.55	1519.9	5746.8	1588.6
.764	900	927.4	918.6	959.7				
.75	1000	1035.5	1008.3	1082.1				
.738	1100	1135.6	1090.6	1197.0				
.727	1200	1234.0	1170.7	1311.1				
.716	1300	1339.2	1255.8	1434.5				
.706	1400	1440.9	1337.7	1555.2				
.697	1500	1537.9	1415.3	1671.5				
.687	1600	1651.9	1506.3	1809.7				

Table 4 : Pressure volume calculations of Ni.

Nickel					
	Pressure P (Kbar)				
V/V_0	Exp. [21]	K. D.	Morse Milstein [1]	Morse Girifalco [19]	Morse Flahive [18]
.993	0	13.3	13.48	10.3	-7.1
.948	100	113.5	121.4	109.2	88.6
.912	200	215.4	240.6	208.9	184.9
.882	300	318.8	369.4	309.2	281.8
.858	400	416.0	496.7	4.02.9	372.2
.836	500	518.4	636.6	501.1	466.9
.816	600	624.1	786.5	601.9	564.1
.799	700	724.7	934.0	697.4	656.1
.784	800	822.7	1081.8	790.1	745.4
.77	900	922.7	1236.7	884.4	836.2
.757	1000	1023.8	1396.9	979.3	927.6
.745	1100	1124.8	1560.4	1073.9	1018.6
.734	1200	1224.4	1725.0	1166.8	1108.6
.724	1300	1321.1	1888.0	1256.9	1194.7
.714	1400	1424.3	2064.9	1352.8	1286.9

In case of Copper, at high relative volume the computed results of P-V calculation using Morse potentials [19] are fairly close with experimental results [21] but at low relative volume Morse potential results are very far from experimental results. At relative volume 0.933 the deviation of experimental results with theoretical results are 0.1% in case of Morse [19] and 13% in case of K. D. potential but at .686 relative volume these deviations are 8.4% in case of Morse and 0.52% in case of K. D. potential. In case of Silver, the deviation between experimental and theoretical results are 4.1% in case of Morse [19] and 9.5% in case of K. D. potential at high relative volume 0.918 but at low relative volume 0.664 these deviations are 2.6% in case of K. D. potential and 14.1% in case of Morse [19] potential.

From Table 3, at high relative volume 0.943 the deviation between experimental and theoretical results of Gold are 19% in case of K. D. potential and 3.72% in case of Morse Potential [18] but at low relative volume .687 these deviations are 3.24% in case of K. D. potential and 13.1% in case of Morse potential. As discussed previously, in case of Aluminum the experimental results are not available but the results of K. D. potential and Morse potential [18] are fairly match. In case of Nickel at high relative volume 0.948 the deviation between experimental and theoretical results are 13.5% for K. D. potential and 9.2% for Morse potential [19] but at low relative volume 0.714 these deviations are 1.72% for K. D. potential and 3.37% for Morse potential [19].

These studies also show that computed results of three Morse potentials are not similar however the computed results of Morse potential used and developed by Girifalco *et. al.* [19] and Morse potential developed by Flahive *et. al.* [18] are not too differ but the results of Morse potential developed by Milstein [1] are very far from other two Morse potentials. Milstein [1] also calculated P-V calculations (only three values of relative volume) of many cubic metals using Morse potential as an interaction between atoms and compared these results with experimental results (extrapolated to 0 ^{0}K) of sock-wave measurements of McQueen *et. al.* [21]. Representation of anharmonic effect in metals by Morse function become fairly poor, such conclusions are found by Milstein [1]. Our study also gives same conclusion.

Figure 1 represents the results of P-V calculation using K. D. and Morse potential [19] in graphical form for Copper. This plot show that overall computed results of P-V calculations by K. D. potential are better match with experimental results [21] in comparison to computed results of Morse potential.

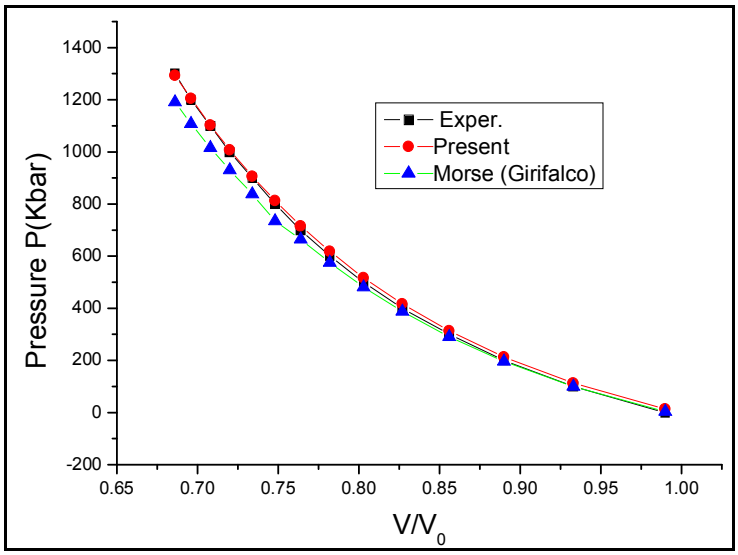

Fig. 1: Comparative result of K. D. potential and Morse Potential for Copper.

5. CONCLUSION

This comparative study gives the theoretical results of P-V calculation using K. D. potential and Morse potentials. We compare these results with experimental results of McQueen *et. al.* [21] and show that computed results of K. D. potential are good match with experimental results [21]. In case of BCC metals, the similar conclusions were found by Kuchhal *et. al.* [17]. Thus these studies show that the two body potential as developed by Kuchhal and Dass [17] is better potential in comparison to Morse potential, which is previously developed by different investigators [1,18,19]. In few cases computed results of Morse potential are better than the K. D. potential but overall results show that the computed results of P-V calculations by K. D. potential are better than the computed results of Morse potential.

REFERENCES

[1] F. Milstein; "Morse function description of anharmonicity in pressure-volume relations of cubic metals", Phys. Status Solidi. B, Vol. 48(2), pp. 681- 688, 1971.

[2] K. P. Thakur; "Mechanical behavior of FCC and BCC metals and their stability under hydrostatic compressive and tensile stresses", J. Phys. F, Vol. 15(12), pp. 2421-2443, 1985.

[3] S. Chantasiriwan and F. Milstein; "Higher order elasticity of cubic metals in the embedded-atom method", Phys. Rev. B. Vol. 53(21), pp. 14080-14088, 1996.

[4] S. Chantasiriwan and F. Milstein" Embedded atom models of 12 cubic metals incorporating second and third-order elastic-moduli data", Phys. Rev. B, Vol. 58(10), pp. 5996, 1998.

[5] Y.O. Ciftci and K. Colankoglu; "Embedded atom method for theoretical strength and stability of some fcc metals", Acta Physica Polonica A., Vol. 100(4), pp. 539-551, 2001.

[6] Y.O. Ciftci, K. Colakoglu, S. Kazanc and S. Ozgen; "The effect of pressure on the elastic constants of Cu, Ag and Au: a molecular dynamics study", Central European journal of physics, Vol. 4(4), pp. 472-480, 2006.

[7] M. Matthew, Armentrout and A. Kavner; "A new high pressure and temperature equation of state of fcc cobalt", J. Appl. Phys., Vol. 118(19), pp. 194904, 2015.

[8] X.D. Dai, Y. Kong, J.H. Li and B X. Liu, "Extended Finnis Sinclair potential for bcc and fcc metals and alloys", J. Phys. Cond. Matter, Vol. 18(19), pp. 4527-4542, 2006.

[9] S.H. Shim, S.D. Thomas and T. Kenichi; "Equation of state of gold and its application to the phase boundaries near 660 km depth in Earth's mantle", Earth and Planetary Scie. Lett., Vol. 203(2), pp. 729-739, 2002.

[10] X. Zheng; "Many body effect on equation of state of solid Ar_4", ICEMEE, IOP Conf. Series Earth and Environment Science, Vol. 295(3), pp. 032041, 2019.

[11] A. Dewaele, P. Loubeyre and M. Mezouar; "Equation of state of six metals above 94 GPa", Phys. Rev. B, Vol. 70(9), pp. 094112, 2004.

[12] Vikram Singh and B.K. Sharma; "Second order elastic constants of Nickel, Gold and Silver", IRJET, Vol. 7(4), pp. 2656-2660, 2020.

[13] Vikram Singh; "Second order elastic constants of copper and aluminum", Science phenomenon, Vol. 1(9), pp. 40-45, 2016.

[14] Vikram Singh and B.K. Sharma; "Third order elastic constants & pressure derivatives of second order elastic constant of some FCC metals", IJSRDV8I20433, Vol. 8(2), pp. 377-380, 2020.

[15] Vikram Singh and B.K. Sharma; "Third order elastic constants and pressure derivatives of second order elastic constant of copper and aluminum", Jour. Pure Appl. and Indu. Phys., Vol 10(4), pp. 1-6, 2020.

[16] Vikram Singh; "Strength and stability of copper using simple two body potential", IJSER, Vol. 4(10), pp. 117-122, 2016.

[17] P. Kuchhal and N. Dass; "Pressure-volume calculation in bcc metals using Born stability criteria", Pramana Jour. of Phys., Vol. 53 (4), pp. 783-794, 1999.

[18] P.G. Flahive and W.R. Graham; "Pair potential calculations of single atom self-diffusion activation energies", Surf. Sci., Vol. 91, pp. 449-462, 1980.

[19] L.A. Girifalco and V.G. Weizer; "Application of the Morse potential function to cubic metals", Phys. Rev. Vol. 114(3), pp. 687-690, 1959.

[20] C. Kittel; "Introduction to solid state physics", John Wiley, New York, 1971.

[21] R.G. McQueen and S.P. Marsh; "Equation of state for nineteen metallic elements from shock wave measurements to two mega bars", J. Appl. Phys. Vol. 31(7), pp. 1253-1269, 1960.