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Mechanical Behavior of FCC Metals using Two Body Potential

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Abstract: ***Mechanical properties such as Bulk modulus, Third order elastic constants, pressure derivatives of second order elastic constants and first pressure derivative of Bulk Modulus of many FCC metals such as Copper, Aluminum, Nickel, Silver and Gold are carried out by taking K. D. potential. Potential parameters of these FCC metals are calculated by taking experimental values of lattice parameter and second order elastic constants. Computed results of these mechanical properties are compared with experimental and calculated results of other investigators. Our calculated results are fairly well agreement with experimental results in comparison to computed results of other workers for all FCC metals except Gold.***
Keywords: Two body potential, Bulk Modulus, Elastic constants, Pressure derivatives.

I. INTRODUCTION

Mechanical properties of cubic metals play an important role in solid state physics. Mechanical properties such as higher order elastic constants and P-V calculations of cubic metals described nonlinear elastic behavior of solid. Elastic constants are of interest in solid state physics since they represent the many anharmonic properties of materials such as thermal expansion, Gruneisen parameters, specific heat etc. by calculating higher order elastic constants, these anharmonic properties can be estimated. Many workers [1-24] have calculated different mechanical properties of cubic metals taking different types of two body and many body potentials. Taking Morse potential, Lincoln et al [1], Girifalco et al [2], and Singh et al [3-5] have estimated second and third order elastic constants of many cubic metals. Temperature dependency of elastic constants has been estimated by Telichko et al [6] and Singh [7]. Golesorkhtabar et al [8] and Dai et al [9] have evaluated elastic constants of cubic metals and alloy. Using extended generalized exponential potential, Verma et al [10, 11] estimated TOEC and pressure derivatives of SOEC of many cubic metals. Lubarda l [12] has calculated third order elastic constants of cubic metals using self consistent method from the linear theory. Blaschke [13] has briefly reviewed strategies of calculating effective isotropic second and third order elastic constants of single crystal. Third order elastic constants for many materials have been determined experimentally [14]. Effect of pressure on mechanical properties such as elastic constants and Bulk Modulus of many cubic metals have been investigated by Ciftci et al [15]. They used modified many body Morse potential function in the framework of M D simulation. Using ab initio density function theory, Wang et al [16] have calculated second, third and fourth order elastic constants of Cu, Al, Au and Ag. Using three ab initio codes Xiaoqing [17] recently obtained the complete set of third order elastic constants of FCC nickel. These studies show that calculations of mechanical properties, such as elastic constants, bulk modulus and pressure derivatives of elastic constant and bulk modulus of FCC metals are active field in present time. Thus the reason cited above it's important to calculate mechanical properties such as bulk modulus, third order elastic constants and pressure derivatives of second order elastic constants and bulk modulus of cubic metals. Recently Singh and coworkers [18-23] estimated many mechanical properties such as second order elastic constants, third order elastic constant, pressure derivatives of second order elastic constants and theoretical strength of many FCC metals using two body potential which is proposed by Kuchhal et al [24]. This potential has two adjustable parameters and three unknown parameters which are calculated by taking experimental values of some physical quantity. By taking experimental values of lattice parameter and second order elastic constant, Kuchhal et al [24] calculated these parameters for BCC metals and by taking experimental values of lattice parameter, bulk modulus and cohesive energy as an input data, Singh and coworkers [18,19] calculated these parameters for many FCC metals. Mechanical properties of FCC metals are carried out recently by Singh and coworker [18-21] by using K. D. potential. The parameters of K. D. potential are calculated by taking experimental values of lattice parameter, bulk modulus and cohesive energy. In this paper we again estimate mechanical properties such as third order elastic constant and pressure derivatives of second order elastic constants and bulk modulus of Cu, Al, Ni, Ag and Au by taking same K. D. potential but the parameters of this potential are estimated by taking experimental values of lattice parameter and second order elastic constants. Thus purpose of present work is to compare the calculated results of mechanical properties of FCC metals using K. D. potentials which are developed by Singh and coworker [18,19] and Kuchhal et al [24].

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II. TWO BODY POTENTIAL

Kuchhal and Dass [24] proposed a simple two body potential for cubic metals. This potential given as

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

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

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

Where all 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.

Kuchhal et al [24] calculated potential parameters of BCC metals by taking experimental values of lattice parameter and second order elastic constants. For evaluation of potential parameters, we are using the same method which is used and developed by Kuchhcal et al [24]. Detail of this method is available in reference [24] so we are not giving procedure of method. For this purpose the experimental values [25] of lattice constant and second order elastic constants for Copper, Aluminum, Nickel, Silver and Gold are shown in table 1.

elements	Lattice parameter (Å)	C_{11} (10^{12} dyne/cm^2)	C_{12} (10^{12} dyne/cm^2)
Copper	3.6153	1.762	1.249
Aluminum	4.049	1.143	.619
Nickel	3.5238	2.612	1.508
Silver	4.0856	1.315	.973
Gold	4.0783	2.016	1.697

Table 1 experimental value [25] of lattice parameter and second order elastic constants.

III. MECHANICAL PROPERTIES OF CUBIC METALS

Expression for bulk modulus is given as

$B.M. = V\frac{\partial^2 E}{\partial V^2}$

Expressions for third elastic constants C_{111} and C_{112} and C_{123} are given as [10]

$c_{111} = \frac{ua^4}{2V}\sum_{l_1}\sum_{l_2}\sum_{l_3} l_1^6 \frac{d^3\emptyset}{(dr^2)^3}$

Where a (= a_1 = a_2 = a_3) is lattice parameter which is shown in table 1. This equation transforms to represent C_{112} and C_{123} when l_1^6 in the said equation is replaced by $l_1^4 l_2^2$ and $l_1^2 l_2^2 l_3^2$ respectively. In these equations u gives number of atoms per unit cell which is four for FCC metals, V gives atomic volume and E gives the energy per atoms.

Pressure derivatives of second order elastic constants and first pressure derivative of bulk modulus are given as [24]

$C'_{11} = \frac{dC_{11}}{dp} = -\frac{2C_{11} + 2C_{12} + C_{111} + 2C_{112}}{C_{11} + 2C_{12}}$

$C'_{12} = \frac{dC_{12}}{dp} = -\frac{-C_{11} - C_{12} + C_{123} + 2C_{112}}{C_{11} + 2C_{12}}$

$B'_T = \frac{1}{3}(C'_{11} + 2C'_{12})$

Where C_{11} and C_{12} are second order elastic constants which are shown in table 1.

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IV. RESULTS AND DISCUSSION

Calculated potential parameters of all FCC metals are shown in table 2. Table 3 gives computed values of bulk modulus and third order elastic constant of Cu, Al, Ni, Ag and Au. Table 4 gives pressure derivatives of second order elastic constant and pressure derivatives of bulk modulus. Table 3 and table 4 also give experimental values [25-29] of these mechanical properties along with calculated results of other workers [20, 21, 30-32].

Elements	Adjustable parameters		Unknown parameters		
	m	n	p (cm^{-m})	A (erg. cm^{n})	B (erg)
Copper	1	5	$2.8866x10^{8}$	$2.4909x10^{-50}$	$3.3115x10^{-9}$
	1	7	$3.4589x10^{8}$	$2.4392x10^{-65}$	$2.0365x10^{-8}$
Aluminum	5	2	$2.2744x10^{38}$	$4.3596x10^{-29}$	$4.8245x10^{-12}$
	2	2	$1.1465x10^{16}$	$4.3833x10^{-29}$	$8.5688x10^{-10}$
Nickel	1	7	$5.057x10^{8}$	$5.0944x10^{-66}$	$1.5613x10^{-7}$
	3	3	$3.5799x10^{23}$	$3.8968x10^{-36}$	$4.4359x10^{-11}$
Silver	1	5	$2.392x10^{8}$	$6.9542x10^{-50}$	$3.3045x10^{-9}$
	1	7	$2.9997x10^{8}$	$7.7215x10^{-65}$	$2.3375x10^{-8}$
Gold	1	5	$2.1684x10^{8}$	$2.2897x10^{-49}$	$6.1181x10^{-9}$
	2	5	$5.0366x10^{15}$	$8.5408x10^{-50}$	$2.3283x10^{-10}$

Table: - 2 Computed potential parameters of FCC metals at different values of adjustable parameters.

We are carried out all results of mechanical properties of FCC metals for two sets of adjustable parameters. Computed results of third order elastic constants and bulk modulus are show in table2. Computed results of adjustable parameters m = 1, n= 5 and m = 2, n = 2 for Copper and Aluminum give fairly good match with Experimental results [27]. In case of Copper and Aluminum, computed results of C_{111} are better match with experimental results [27] in comparison to Singh [20] results of K. D. potentials. Deviation of theoretical and experimental results of C_{111} 14% and 10.86% for Copper and Aluminum in present potential however 18.8% and 14.44% in case of Singh [20] results. Similarly computed results of this K. D. potential of C_{112} for Copper is close with experimental results [27] in comparison to Singh [20] K. D. potential but in case of Aluminum these computed results are poor match with Experimental results [27] with respect to computed results of Singh [20]. All computed results of C_{111} and C_{112} for Ni, Ag and Au in this study are poor match with experimental results [26,27] in comparison to Singh et al [21] computed results of K. D. potential expect computed results of C_{112} for Silver. It is interesting that the present potential gives very poor results of C_{111} and C_{112} in case of Gold. In case of C_{123}, the agreement between theoretical and experimental result are very poor. Our results show C_{123} is positive for all FCC metals but the experimental results for Copper, Nickel and Gold are negative and for Aluminum and Silver, are positive. Lincoln et al [31] detail explained why the value of C_{123} of FCC metals is positive. Table 2 also shows that, the computed results of our study are better match with experimental results [26, 27] in comparison to other worker [31, 32]. Table 2 also gives the calculated results of bulk modulus along with experimental results [25] and show that these results are better match with experimental results [25].

Elements	Adjustable parameters		Mechanical properties (10^{12} dyne/cm^2)			
	m	n	C_{111}	C_{112}	C_{123}	B.M.
Copper	1	5	-10.93	-7.9	.912	1.42
	1	7	-8.87	-7.28	.76	
	Experimental [25,27]		-12.71	-8.14	-.5	1.37
	Singh (K. D. potential) [20]		-15.1	-7.66	.042	-
	Other [31]		-11	-7.49	.77	-
Aluminum	5	2	-9.89	-5.34	.114	.7937
	2	2	-12.72	-6.75	.115	
	Experimental [25,27]		-14.27	-4.08	.32	.722
	Singh (K. D. potential) [20]		-12.21	-6.31	.0113	-
	Other [31]		-5.92	-3.86	.448	-
Nickel	1	7	-27.81	-16.03	.292	1.876
	3	3	-22.72	-13.17	.416	
	Experimental [25,26]		-20.4	-10.3	-2.1	1.86
	Singh (K. D. potential) [21]		-21.12	-10.72	.0584	
	Other [32]		-17.896	-11.42	.814	
Silver	1	5	-7.124	-5.47	.84	1.087
	1	7	-5.05	-4.88	.672	
	Experimental [25,27]		-8.43	-5.29	.4874	1.007
	Singh (K. D. potential) [21]		-8.47	-4.48	.075	
	Other [31]		-9.322	-6.29	1.89	
Gold	1	5	-5.71	-6.19	2.11	1.8033
	2	5	-4.06	-6.426	1.62	
	Experimental [25,27]		-17.29	-9.22	-2.33	1.732
	Singh (K. D. potential) [21]		-18.14	-9.39	.094	
	Other [31]		-18.42	-11.1	.6141	

Table: - 3 Computed mechanical properties of FCC metals with experimental result.

Table 4 gives calculated values of pressure derivatives of second order elastic constants (C_{11}' and C_{12}') and first pressure derivatives of bulk modulus (B_T') for Cu, Al, Ni, Al and Au. These results show that the computed results of present study are not good match with experimental results [27-30] in comparison to Singh and coworker [20,21] computed results of K. D. potential however in few cases these results are better match with experimental results in comparison to calculated results of other worker [31, 32]. These results also show that, in case of Gold the experimental and theoretical results are very far from each other. This discussion showed that our computed results are not too better results in comparison to the calculated results of Singh and coworker [20,21] however our results are better in comparison to calculated results of other workers [31, 32]. This study further gives a conclusion that the present potential is not suitable for Gold. For other FCC metal this potential gives better results in comparison to other potential which are used by other workers [31, 32].

Above mentioned discussion show that present potential is not too suitable for Gold however for other FCC metals this gives better results. As we are only calculated third order elastic constants, bulk modulus and pressure derivatives of second order elastic constants and bulk modulus and not calculate other mechanical property such as pressure volume calculations. So calculated results of other mechanical properties decided the potential is suitable or not suitable for Gold.

Elements	Adjustable parameters		Mechanical properties		
	m	n	C_{11}'	C_{12}'	B_T'
Copper	1	5	4.86	4.2	4.2
	1	7	4.086	3.95	3.99
	Experimental [27]		5.73	4.98	5.44
	Singh (K. D. potential) [20]		5091	4.4655	4.947
	Other [31]		5.2	4.32	4.62
Aluminum	5	2	7.18	5.2	5.86
	2	2	9.56	6.4	7.4
	Experimental [28,29]		7.02	3.94	5.19
	Singh (K. D. potential) [20]		9.7852	6.3966	7.5261
	Other [31]		4.88	4.06	4.34
Nickel	1	7	9.17	6.38	7.31
	3	3	7.25	5.34	5.98
	Experimental [30]		6.03	4.87	5.26
	Singh (K. D. potential) [21]		6.134	4.5776	5.1104
	Other [32]		5.70	4.58	4.95
Silver	1	5	4.137	3.8	3.91
	1	7	3.14	3.49	3.37
	Experimental [27]		4.859	3.35	4.11
	Singh (K. D. potential) [21]		4.283	3.6768	3.8789
	Other [31]		5.83	4.73	5.09
Gold	1	5	1.9706	2.58	2.38
	2	5	1.754	2.7603	2.42
	Experimental [27]		5.494	4.73	5.21
	Singh (K. D. potential) [21]		5.621	4.3398	4.7669
	Other [31]		6.69	5.19	5.68

Table: - 4 Computed mechanical properties of FCC metals with experimental result.

V. CONCLUSION AND FUTURE WORK

Previous studies [18-23] show that the potential used in this work is very simple and the computed results of many mechanical properties such as second order elastic constant [18,19], third order elastic constants [20,21] and theoretical strength [22,23] of FCC metals are better match with experimental results. Thus these studies show that K. D. potential is better potential for FCC metals in comparison to other two body potential. Kuchhal et al [24] also found same conclusion for estimation of mechanical properties of many BCC metals. Thus it gives us a motivation to calculate mechanical properties of FCC metals using K. D. potential which is used and developed by Kuchhal et al [24] for BCC metals. So in present work we calculate potential parameters of FCC metals and we estimate many mechanical properties of FCC metals. This potential is not give too better results of third order elastic constants and pressure derivatives of second order elastic constants and first pressure derivative of bulk modulus in comparison to computed results of Singh and coworker [20,21]. The computed results of these mechanical properties using present potential are better than the calculated results of other workers [31, 32]. Computed results of bulk modulus in this study are better match with experimental results [25]. In future, we also calculate these mechanical properties of other FCC metals by taking K. D. potential.

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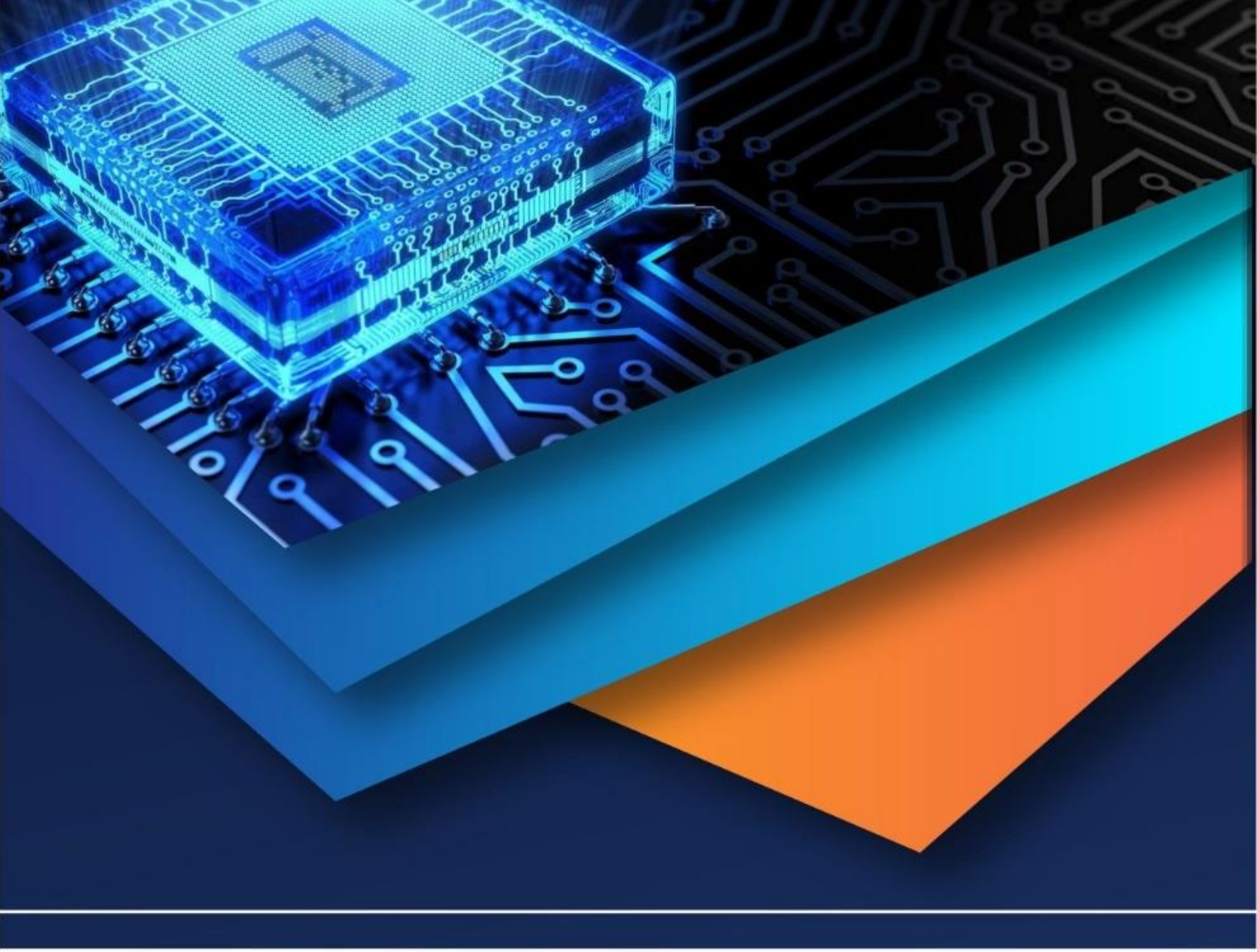

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