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Pressure–volume calculation in bcc metals using Born stability criteria

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Abstract. A simple analytical two-body potential $\phi(r) = -Ar^{-n} + B\exp(-pr^m)$ is considered for P-V calculations in bcc metals using Born stability criteria. It is shown that the stability of bcc metals can be expressed uniquely as a function of a parameter q (discussed in the text). The P-V calculations are done in ten bcc metals. The calculations are compared with the experimental data of shock-wave measurements and also with other potential available. It is found out that the present potential is better than the other two-body potentials in case of bcc metals. Further, the calculations done for TOEC and the first pressure derivative of SOEC are found in good agreement with the reported results.

Keywords. Two-body pair potential; Born stability criteria; second and third order elastic constants; bcc metals.

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1. Introduction

The study of high pressure behaviour of materials has become quite interesting in recent years because of the discovery of new crystal structures and structural phase transitions and also due to many geophysical and technological applications. Moreover, the anharmonicity of solids can be examined by studying the P-V behaviour [1]. The P-V calculations are performed by using the empirical two body interatomic central potential. Though the interatomic forces in solid are admixture of the central, non-central, and many-body forces, even then the use of two-body central force potential is quite successful in the study of many properties of solids [2]. However, it will not be out of place to mention here that band structure methods can also be used for P-V calculations [17].

Max Born [3,4] investigated the conditions under which a crystal lattice will be thermodynamically stable. Necessary condition for the thermodynamic stability of a crystal lattice is that the crystal be mechanically stable with respect to an arbitrary homogeneous deformation. Born [3,4] derived the mathematical expressions for cubic lattices of the Bravis type on the assumption of two-body central potential of a very general nature as $C_{12} > 0$ and $C_{11} - C_{12} > 0$ where C_{ij} represents second order elastic constants of the solid.

Table 1. Input parameters for present potential. Experimental data of C_{11}, a_0 and C_{11}/C_{12} are taken from [6] at 0 K. The values in paranthesis are for logarithmic potential.

Elements	a_0 (Å)	A ($\times 10^{12}$ dyne/cm^2)	C_{11}	q	C_{11}/C_{12}	n			(erg-cm^n)	B (erg)	p (cm^{-m})
Li	3.500		0.1481		1.1867	5	1	3.8794	1.5653×10^{-50}	5.1103×10^{-10}	2.2162×10^{8}
						(2)	(13)	(511.00)	(1.8267×10^{-29})	(1.9265×10^{-13})	(7.3632×10^{-9})
Na	4.3249		0.0815		1.2003	4	1	3.6103	6.0034×10^{-43}	2.1384×10^{-10}	1.7050×10^{8}
						(2)	(11)	(82.140)	(2.6724×10^{-29})	(3.9020×10^{-13})	(3.1513×10^{-83})
K	5.2250		0.0416		1.2199	4	1	3.5105	1.4485×10^{-43}	1.9011×10^{-10}	1.3437×10^{8}
						(2)	(11)	(97.686)	(3.9887×10^{-29})	(3.3039×10^{-13})	(3.7796×10^{-82})
Rb	5.5850		0.0358		1.1807	4	1	3.7214	1.6807×10^{-42}	2.3599×10^{-10}	1.3326×10^{8}
						(2)	(12)	(197.693)	(4.5432×10^{-29})	(2.7216×10^{-13})	(4.4454×10^{-89})
Nb	3.2961		2.4801		1.6209	3	1	2.7481	5.8633×10^{-35}	7.4843×10^{-10}	1.6675×10^{8}
						(2)	(32)	(3.6952×10^{8})	(4.8752×10^{-28})	(8.2120×10^{-13})	(3.2411×10^{-241})
Ta	3.2979		2.6632		1.6839	3	1	2.6315	6.8741×10^{-35}	7.2350×10^{-10}	1.5958×10^{8}
						(2)	(32)	(4.1503×10^{8})	(5.2148×10^{-28})	(8.7405×10^{-13})	(3.3821×10^{-241})
V	3.0352		2.324		1.9471	2	1	2.0813	1.7855×10^{-28}	1.7855×10^{-10}	1.9194×10^{8}
						(2)	(32)	(3.8685×10^{7})	(2.7328×10^{-28})	(1.2933×10^{-12})	(2.5844×10^{-242})
W-α	3.1620		5.3255		2.5984	2	1	2.0813	6.8790×10^{-28}	3.1283×10^{-10}	1.3165×10^{8}
						(2)	(28)	(3.8685×10^{7})	(5.9641×10^{-28})	(1.2933×10^{-12})	(1.4376×10^{-231})
Mo	3.1470		4.5002		2.6025	2	1	2.0776	5.6843×10^{-28}	2.5925×10^{-10}	1.3204×10^{8}
						(2)	(28)	(3.8722×10^{7})	(4.9671×10^{-28})	(1.0769×10^{-12})	(1.4390×10^{-231})
Cr	2.8845		3.500		5.000	3	1	1.5790	1.0850×10^{-34}	2.5395×10^{-10}	1.0948×10^{8}
						(2)	(28)	(5.4269×10^{7})	(2.3385×10^{-28})	(5.3716×10^{-13})	(1.5406×10^{-212})

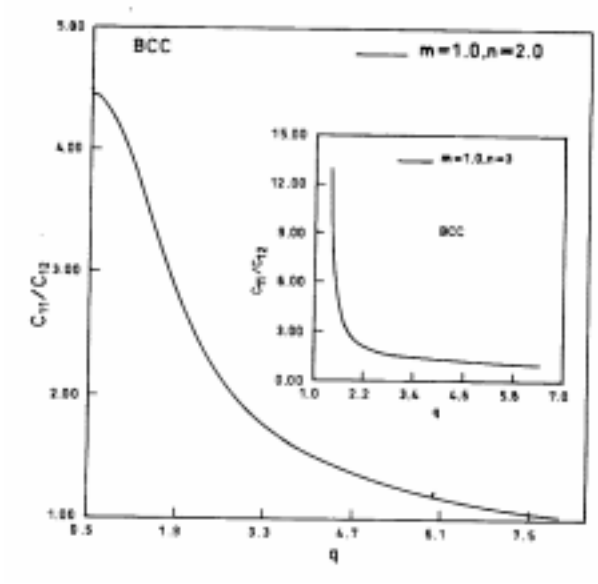

Figure 1. Variation of the ratio of elastic moduli C_{11}/C_{12} with the potential parameter q for bcc lattices according to the present potential for $n = 2$ and $n = 3$.

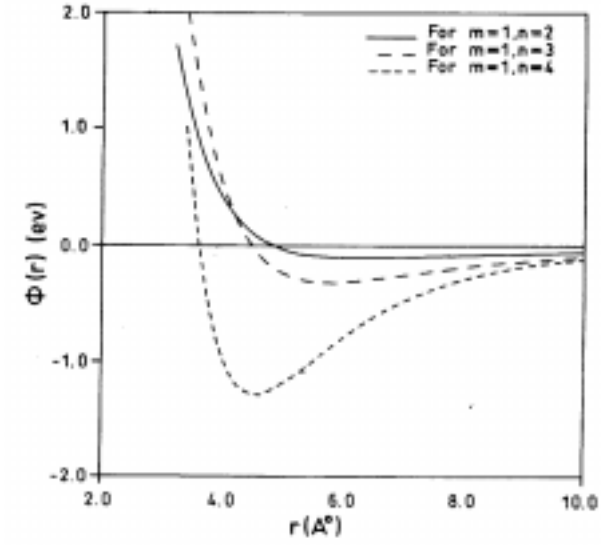

Figure 2. Variation of potential function in case of Mo versus interatomic distance.

Milstein [1,2,5] had clearly shown that generalized Morse potential is unable to give the P-V calculations in case of bcc metals. On the other hand, Thakur [6] had used two-body logarithmic potential for P-V calculations in case of bcc metals but the computed results

are not in good agreement with the shock-wave measurements as is evident from tables 2, 4 and figure 3. Therefore, it can be concluded that the two-body potential so far available are unable to give good P-V data in case of bcc metals.

Hence, the aim of the present paper is to give a suitable two-body potential which can give good results of P-V calculations using Born stability criteria.

2. Theory and procedure

For P-V calculations, we suggest the two-body potential as

$$\phi(r) = Ar^{-n} + B\exp(-pr^m), \tag{1}$$

where A, B and p are positive constants and are expressed in unit of erg.cm^n, erg and cm^{-m}, respectively. r is the distance from a lattice site chosen as the origin to a given lattice site with coordinates specified by the three integers l_1, l_2, l_3 as

$$r = \frac{1}{2}a_0(l_1^2 + l_2^2 + l_3^2)^{1/2}, \tag{2}$$

where a_0 is lattice constant at zero pressure and absolute zero temperature. Since this potential is basically empirical one in nature, there is no limit to the number of different function which can be calculated from a given set of experimental data. Thus, any family of potential function should include relatively short range steep potentials as well as longer-range shallower potentials. Further, the potential parameters, A, B and p are determined by using the experimental values of C_{11}, C_{12} and a_0 keeping m and n as adjustable parameters.

Born criteria for stability of a crystal can be described in terms of mathematical expression as

$$\sum_{l_1}\sum_{l_2}\sum_{l_2} l_1^2 \frac{\mathrm{d}\phi(r)}{\mathrm{d}r^2} = 0. \tag{3}$$

This is the condition of the equilibrium of a crystal in the absence of the external force. Born [3,4] has derived the mathematical expressions for the elastic constant C_{11} and C_{12} for cubic crystal with two-body interatomic interaction and the same can be written for bcc metal as:

$$C_{11} = \frac{a_0}{4}\sum_{l_1}\sum_{l_2}\sum_{l_3} l_1^4 \frac{\mathrm{d}^2\phi(r)}{(\mathrm{d}r^2)^2}, \tag{4}$$

$$C_{12} = \frac{a_0}{4}\sum_{l_1}\sum_{l_2}\sum_{l_2} l_1^2 l_2^2 \frac{\mathrm{d}^2\phi(r)}{(\mathrm{d}r^2)^2}. \tag{5}$$

The summation in (3)-(5) are over all lattice sites (except the origin $l_1 = l_2 = l_3 = 0$) in the crystal.

Table 2. Pressure, P(Kbar), as a function of volume in V, Mo and W-α by using present potential. Exptl. data for V, Mo and W-α are taken from [7].

V				Mo				W-α			
V/V_0	P (exptl.)	P Present	P Others*	V/V_0	P (exptl.)	P Present	P Others*	V/V_0	P (exptl.)	P Present	P Others*
0.995	0.0	7.94	8.0	0.997	0.0	8.01	8.00	0.997	0.0	9.49	9.0
0.940	100	109.09	102	0.962	100	110.02	105	0.967	100	111.83	107
0.898	200	206.54	201	0.934	200	204.24	191	0.942	200	208.50	196
0.862	300	307.62	320	0.910	300	295.31	273	0.918	300	312.42	290
0.831	400	410.45	451	0.887	400	392.74	362	0.898	400	408.35	377
0.806	500	505.99	574	0.866	500	491.48	453	0.879	500	508.27	468
0.783	600	605.46	693	0.849	600	579.02	533	0.862	600	605.66	558
0.763	700	702.24	796	0.832	700	674.08	618	0.847	700	698.46	642
0.744	800	804.22	889	0.817	800	764.81	697	0.832	800	798.28	732
0.727	900	904.76	964	0.803	900	855.79	773	0.819	900	890.93	813
0.712	1000	1000.58	1021	0.788	1000	961.62	856	0.807	1000	981.91	889
0.698	1100	1099.51	1066	0.776	1100	1050.40	922	0.795	1100	1078.51	967
0.684	1200	1205.44	1103	0.764	1200	1145.87	987	0.784	1200	1172.33	1039
				0.754	1300	1230.07	1040	0.774	1300	1262.30	1104
				0.744	1400	1318.78	1091	0.764	1400	1357.00	1169
				0.734	1500	1412.26	1140	0.754	1500	1456.72	1231
								0.746	1600	1540.31	1280
								0.738	1700	1627.08	1327
								0.729	1800	1730.08	1377
								0.721	1900	1825.48	1420

*Calculated from logarithmic potential [6].

Table 3. Pressure P (Kbar) as a function of volume in Li, Na, K and Rb by using present potential. Exptl. data for all of these elements are taken from [8].

	Li			Na			K			Rb		
V/V_0	P (Exptl.)	P (Present)	P Others*	P (Exptl.)	P (Present)	P Others*	P (Exptl.)	P (Present)	P Others*	P (Exptl.)	P (Present)	P Others*
0.9200	6.5	12.973	13.27	3.2	7.17	7.46	1.3	3.61	3.74	0.8	3.10	3.28
0.8800	13.5	21.610	22.26	7.4	12.04	12.77	3.4	6.04	6.37	2.2	5.38	5.58
0.8400	22.3	32.070	33.17	12.6	18.05	19.48	5.9	9.03	9.67	3.9	8.09	8.44
0.8000	32.9	44.740	46.29	19.1	25.47	27.93	9.0	12.71	13.78	6.1	11.45	11.98
0.7600	46.0	60.090	61.92	27.2	34.67	38.67	12.9	17.26	18.88	8.8	15.63	16.34
0.7200	62.3	78.670	80.38	37.4	46.15	51.81	17.7	22.89	25.20	12.2	20.87	21.65
0.6800	82.8	101.140	102.05	50.6	60.54	68.34	23.7	29.93	32.99	16.6	27.47	28.09
0.6400	108.9	128.270	127.32	67.9	78.68	88.84	31.5	38.76	42.52	22.4	35.84	35.84
0.6000	142.7	160.920	156.66	90.9	101.76	114.15	41.7	49.93	54.16	30.0	46.53	45.12
0.5600	187.3	199.980	190.59	122.4	131.37	145.26	55.4	64.18	68.32	40.4	60.33	56.10
0.5200	247.6	246.170	229.64	167.1	169.77	183.41	74.0	82.55	85.48	55.1	78.33	69.36
0.4800				232.7	220.20	230.07	103.7	106.51	106.28	76.6	102.13	84.97
0.4400				334.5	287.40	287.18	139.4	138.18	131.49	109.5	134.07	103.49
0.4000							200.0	180.73	162.22	163.6	177.74	125.53
0.3800							243.7	207.51	180.14	–	205.62	138.16
0.3600										261.2	238.77	152.14

*Calculated from logarithmic potential [6].

Table 4. Pressure, P(kbar), as a function of volume in Cr, Nb and Ta by using present potential. Exptl. data from [7] for Cr and [9] for Nb and Ta.

Cr				Nb				Ta			
V/V_0	P (exptl.)	P Present	P Others*	V/V_0	P (exptl.)	P Present	P Others*	V/V_0	P (exptl.)	P Present	P Others*
0.996	0.0	6.59	6.57	1.000	0.0	0.00	0.00	1.0000	0.0	0.00	0.00
0.933	100	125.96	125.89	0.9485	100	107.63	97.01	0.9543	100	98.87	90.36
0.890	200	227.51	230.67	0.9072	200	215.13	189.72	0.9169	200	197.07	175.94
0.856	300	322.19	327.89	0.8730	300	321.85	288.86	0.8852	300	295.07	266.67
0.827	400	414.94	417.69	0.8436	400	428.98	396.12	0.8576	400	313.42	364.85
0.803	500	501.38	493.13	0.8180	500	535.89	506.11	0.8334	500	491.23	467.45
0.782	600	585.21	556.92	0.7953	600	642.93	616.38	0.8172	600	563.53	544.34
0.764	700	663.89	607.81	0.7751	700	749.20	719.08	0.7992	700	687.25	673.09
0.748	800	739.70	648.73	0.7567	800	856.19	813.21	0.7744	800	785.37	768.99
0.734	900	810.97	680.34	0.7400	900	962.65	895.94	0.7580	900	884.06	857.39
0.720	1000	887.29	707.39	0.7247	1000	1068.85	967.05	0.7430	1000	981.98	935.84
				0.7105	1100	1175.57	1027.27	0.7291	1100	1079.88	1004.60
				0.6974	1200	1281.62	1076.75	0.7161	1200	1178.22	1064.07
				0.6852	1300	1387.53	1116.85	0.7040	1300	1276.14	1114.07
				0.6738	1400	1493.23	1148.67	0.6926	1400	1374.47	1156.20
				0.6632	1500	1597.80	1173.12	0.6820	1500	1471.59	1190.23
				0.6532	1600	1702.43	1191.51	0.6719	1600	1569.60	1217.89
				0.6437	1700	1807.56	1204.72	0.6623	1700	1668.04	1239.74
				0.6348	1800	1911.47	1213.33	0.6523	1800	1776.42	1257.77
								0.6447	1900	1863.04	1268.22
								0.6366	2000	1959.62	1276.25
								0.6288	2100	2057.03	1280.98
								0.6214	2200	2153.65	1282.73
								0.6144	2300	2249.02	1281.97

*Calculated from logarithmic potential [6].

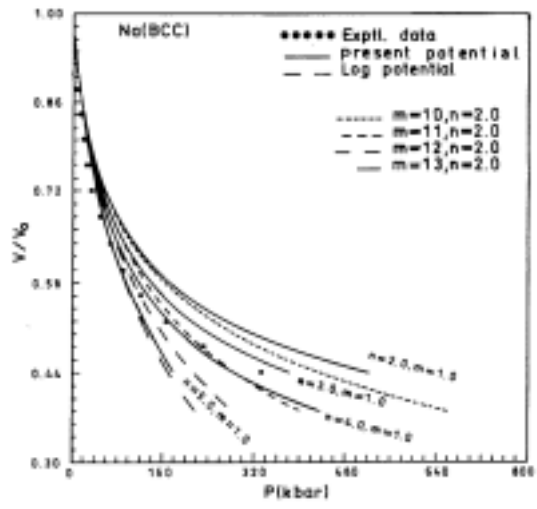

Figure 3. Comparison of the pressure-volume behaviour of sodium obtained from the present potential with (i) different n and (ii) from the logarithmic potential with different m together with the experimental data.

From (1)

$$\frac{\mathrm{d}\phi(r)}{\mathrm{d}r^2} = \frac{1}{2}\left[\frac{nA}{r^{n+2}} - Bmpr^{m-2}\exp(-pr^m)\right], \tag{6}$$

and

$$\frac{\mathrm{d}^2\phi(r)}{(\mathrm{d}r^2)^2} = \frac{1}{4}\left[\frac{-n(n+2)A}{r^{n+4}} - Bm(m-2)pr^{m-4}\exp(-pr^m) + Bm^2p^2r^{2m-4}\exp(-pr^m)\right] \tag{7}$$

The relation for C_{11} and C_{12} can be expressed uniquely, if we define the following new parameters:

$$A' = A(a_0/2)^{-n}, \tag{8}$$

$$q = p(a_0/2)^m, \tag{9}$$

and

$$\rho = (l_1^2 + l_2^2 + l_3^2)^{1/2}. \tag{10}$$

Substituting (8)-(10) into (6) and (7), we get

$$\frac{\mathrm{d}\phi(r)}{\mathrm{d}r^2} = \frac{2}{a_0^2}\left[\frac{nA'}{\rho^{n+2}} - Bmq\rho^{m-2}\exp(-q\rho^m)\right], \tag{11}$$

and

$$\frac{\mathrm{d}^2\phi(r)}{(\mathrm{d}r^2)^2} = \frac{4}{a_0^4}\left[\frac{-n(n+2)A'}{\rho^{n+4}} - Bm(m-2)q\rho^{m-4}\exp(-q\rho^m) + Bm^2q^2\rho^{2m-4}\exp(-q\rho^m)\right]. \tag{12}$$

From (3) and (11), we get

$$A' = \frac{Bm}{n}\frac{\mathrm{d}(l_i, q)}{\mathrm{e}(l_i)}, \tag{13}$$

where

$$d(l_i, q) = \sum_{l_1}\sum_{l_2}\sum_{l_3} l_1^2 q\rho^{m-2}\exp(-q\rho^m), \tag{14}$$

$$\mathrm{e}(l_i) = \sum_{l_1}\sum_{l_2}\sum_{l_3} l_1^2\rho^{-(n+2)}. \tag{15}$$

From (4), (5) and (12), we get

$$C_{11} = \frac{Bm}{a_0^3}\left[\frac{-(n+2)\mathrm{d}(l_i q) f(l_i)}{\mathrm{e}(l_i)} + g(l_i, q)\right], \tag{16}$$

$$C_{12} = \frac{Bm}{a_0^3}\left[\frac{-(n+2)\mathrm{d}(l_i q) h(l_i)}{\mathrm{e}(l_i)} + k(l_i, q)\right], \tag{17}$$

where

$$f(l_i) = \sum_{l_1}\sum_{l_2}\sum_{l_3} l_1^4 \rho^{-(n+4)}, \tag{18}$$

$$g(l_i, q) = \sum_{l_1}\sum_{l_2}\sum_{l_3} l_1^4 q\rho^{m-4} \exp(-q\rho^m)[mq\rho^m - (m-1)], \tag{19}$$

$$h(l_i) = \sum_{l_1}\sum_{l_2}\sum_{l_3} l_1^2 l_2^2 \rho^{-(n+4)}, \tag{20}$$

$$k(l_i, q) = \sum_{l_1}\sum_{l_2}\sum_{l_3} l_1^2 l_2^2 q\rho^{m-4} \exp(-q\rho^m)[mq\rho^m - (m-1)]. \tag{21}$$

In considering the summation in (16) and (17), we have taken 89,460 atoms (except origin $l_1 = l_2 = l_3 = 0$) in the bcc crystals. Further, the summations are accomplished by summing over integer value of l_1, l_2 and l_3 subject to the restriction that l_1, l_2 and l_3 are either all even or all odd. Although the atoms interact through a two-body potential function $\phi(r)$, each atom interacts with all the other atoms in the lattice, the contributions of these interaction are taken into account over a sufficiently large number of lattice sites.

Before applying the present potential in bcc metals, we have to check the Born stability criteria i.e. $C_{12} > 0$ and $C_{11} - C_{12} > 0$.

Since Bm/a_0^3 is positive for the present potential, the first stability condition $C_{12} > 0$ is satisfied provided the function in the bracket in (17) is also positive. In present study, this function is evaluated for bcc lattice and has been found to be positive when (i) $q > 0.3$ for $n = 2$ and $m = 1$, (ii) $q > 1.29$ for $n = 3$ and $m = 1$ and (iii) $q > 3.1$ for $n = 4$ and $m = 1$. The second condition for Born stability criteria is expressed uniquely as a function of q as

$$\frac{C_{11}}{C_{12}} = \frac{[(n+2)\mathrm{d}(l_i, q) f(l_i)/e(l_i)] - g(l_i, q)}{[(n+2)\mathrm{d}(l_i, q) h(l_i)/e(l_i)] - k(l_i, q)} \tag{22}$$

The ratio C_{11}/C_{12} is determined as a function of q. The ratio C_{11}/C_{12} versus q is plotted in figure 1 for $n = 2$ and $n = 3$ keeping $m = 1$ in both the cases. Figure 1 shows that C_{11}/C_{12} is evidently greater than unity upto (i) $q = 8.53$ for $n = 2$ and $m = 1$, (ii) $q = 6.52$ for $n = 3$ and $m = 1$ and (iii) $q = 5.32$ for $n = 4$ and $m = 1$. The values of C_{11}/C_{12} obtained from the potential lie within the experimental data for all the bcc metals.

Experimental values of the lattice parameter a_0 and the elastic constants C_{11} and C_{12} are listed in table 1 for each bcc metal. For a known value of C_{11}/C_{12}, we can obtain the value of q from (22). Once the value of q is available, one can obtain, the value of B from (16) using the experimental data of C_{11}. The value of A' can then be computed from (13). The value of A' and q give the values of A and p, and can be obtained from (8) and (9) respectively.

3. Pressure–volume calculations

When the crystal is subject to hydrostatic pressure, the lattice parameter a_i all remain equal i.e. $(a_1 = a_2 = a_3 = a)$ and the pressure (at $T = 0$K) is given by

$$P = \frac{1}{2a} \sum_{l_1} \sum_{l_2} \sum_{l_3} l_1^2 \frac{\mathrm{d}\phi(r)}{\mathrm{d}r^2}, \tag{23}$$

with

$$r = \frac{1}{2} a (l_1^2 + l_2^2 + l_3^2)^{1/2} \tag{24}$$

and the corresponding relative volume is given by

$$V/V_0 = (a/a_0)^3. \tag{25}$$

Thus, the pressure can be calculated from (23). In tables 2, 3 and 4, the calculated values of P versus V/V_0 in case of 10 bcc metals are compared with the experimental data along with the logarithmic potential [6] by using the parameter needed from table 1. The experimental pressure data alongwith V/V_0 are taken from McQueen and Marsh [7] for V, Mo, W-α and Cr; from Rice [8] for Li, Na, K, and Rb; and from McQueen *et al* [9] for Nb and Ta.

The pressure is calculated from the present potential as well as from the logarithmic potential [6] using optimum value of m and n and the results are reported in table 3 for Li, Na, K and Rb; in table 4 for Cr, Nb and Ta; and in table 2 for V, Mo, W-α along with the available experimental data. The calculated results from the present potential are in very good agreement with the experimental data in the whole range of compression in each bcc metal as is evident from the tables 2–4.

Theoretical P-V calculations are sensitive to the parameters m and n involved in the present potential. For fixed value of $m = 1$, when n is varied from 2 to 5 then it is observed that as n increases, the pressure decreases at high compression whereas at lower compression the effect of n is small as shown in figure 3.

4. The third order elastic constant (TOEC$_s$) and pressure derivative of second order elastic constant (SOEC$_s$)

For a cubic crystal, there are three independent second order elastic constants, namely, C_{11}, C_{12}, and C_{14} and six independent third order elastic constants $C_{111}, C_{112}, C_{123}, C_{456}, C_{144}$ and C_{166}. In the central force model, the elastic constants follow the Cauchy relations:

$$C_{12} = C_{44} \tag{26}$$

$$C_{112} = C_{166} \tag{27}$$

$$C_{123} = C_{456} = C_{144}. \tag{28}$$

Hence, we need C_{11} and C_{12} as SOEC and C_{111}, C_{112} and C_{123} as TOEC for further calculations. The expression for the SOEC$_s$ is given by (4) and (5) and third order elastic constants are given below as:

$$C_{111} = \frac{a^3}{8} \sum_{l_1} \sum_{l_2} \sum_{l_3} l_1^6 \frac{\partial^3 \phi(r)}{(\partial r^2)^3}, \tag{29}$$

$$C_{112} = \frac{a^3}{8} \sum_{l_1} \sum_{l_2} \sum_{l_3} l_1^4 l_2^2 \frac{\partial^3 \phi(r)}{(\partial r^2)^3}, \tag{30}$$

and

$$C_{123} = \frac{a^3}{8} \sum_{l_1} \sum_{l_2} \sum_{l_3} l_1^2 l_2^2 l_3^2 \frac{\partial^3 \phi(r)}{(\partial r^2)^3}. \tag{31}$$

The values of TOEC$_s$ can be computed from (29) to (31). Further, the pressure derivatives of SOEC$_s$ can be calculated which are given by the following relations [10].

$$C'_{11} = \frac{\partial C_{11}}{\partial P} = -\frac{2C_{11} + 2C_{12} + C_{111} + 2C_{112}}{C_{11} + 2C_{12}} \tag{32}$$

and

$$\mathrm{C}'_{12} = \frac{\partial \mathrm{C}_{12}}{\partial P} = \frac{-\mathrm{C}_{11} - \mathrm{C}_{12} + \mathrm{C}_{123} + 2\mathrm{C}_{112}}{\mathrm{C}_{11} + 2\mathrm{C}_{12}}. \tag{33}$$

Moreover, the isothermal bulk modulus, B_T, and its first pressure derivative, B'_T, can also be calculated from the relations given below

$$B_T = \frac{1}{3}(C_{11} + 2C_{12}) \tag{34}$$

and

$$B'_T = \frac{1}{3}(C'_{11} + 2C'_{12}) \tag{35}$$

The TOEC$_s$ C_{111}, C_{112} and C_{123} first pressure derivative of SOEC$_s$, and B'_T are calculated for 10 bcc metal using our potential and are listed in table 5. The experimental values of B'_T are also listed in the same table for comparison. We have also reported the pressure variation of isothermal bulk-modulus in table 6 in case of Li and K along with the available data of B_T from other results.

Analytical form of the present potential

The computed potential parameters are used to arrive at a graphical representation of bcc metal, using eq. (1). Figure 2 shows the variation of our potential function versus the interatomic separation r for Mo with different value of m and n. Perusal of figure 2 reveals

Table 5. Third order elastic constants, first pressure derivative of second order elastic constants and isothermal bulk modulus at $T = 0$ K and $P = 0$ kbar.

Elements	C_{111} (kbar)	C_{112} (kbar)	C_{123} (kbar)	C'_{11}	C'_{12}	B'_T
Li	1600	−336	−525	4.35	3.70	3.91 (3.27)[b]
Na	−873 (−928)[a]	−206 (−189)[a]	−302 (−197)[a]	4.54 (4.03)[a]	3.98 (3.53)[a]	4.16 (3.70)[a]
K	−441 (−424)[a]	−99.3 (−88)[a]	−150 (−101)[a]	4.45 (4.31)[a]	3.86 (3.62)[a]	4.06 (3.97)[a]
Rb	−387	95.9	−137	4.63	4.10	4.28 (3.19)[b]
Nb	−23800	−4250	−6050	4.38	3.35	3.39 (4.03)[b]
Ta	−25200	−4310	−6130	4.36	3.26	3.63 (3.58)[b]
V	−20900	−3890	−4370	4.59	3.33	3.75 (3.59)[b]
W	−44400	−7150	−6090	4.66	2.95	3.52 (3.58)[b]
Mo	−37500	−6030	−5130	4.67	2.94	3.52 (3.72)[b]
Cr	−28700	−2590	−4080	5.19	2.00	3.60 (4.75)[b]

[a]Taken from ref. [13]; [b]taken from ref. [14].

Table 6. Variation of B_T with volume at 0 K in Li and K.

Li			K		
V/V_0	B_T (Present)	B_T (Others)[a]	V/V_0	B_T (Present)	B_T (Others)[b]
1.0000	133	123	1.0000	36.6	37.0
0.9850	140	130	0.9928	37.6	38.0
0.9653	150	140	0.9697	41.0	42.0
0.9456	161	149	0.9467	44.6	46.0
0.9259	172	162	0.9236	48.6	50.5
0.9062	184	175	0.9005	53.0	55.5
0.8865	197	191	0.8774	57.8	61.5
			0.8543	63.0	68.5
			0.8312	68.7	76.0
			0.8081	75.0	84.5
			0.7850	81.9	94.0
			0.7619	89.5	105.0

[a]Taken from ref. [15]; [b]taken from ref. [16].

that the variation of m in association with n incur the vertical as well as horizontal shift of potential minima, and hence indicates the inclusion of exchange and correlation effects [11] and the three body effects [12].

5. Conclusion

It is quite clear from the above discussions that the present potential works very well and is successful in representing the P-V calculations in bcc metals, whereas (i) the Morse generalized potential can not be used at all and (ii) the results obtained from logarithmic potential are not in good agreement with the experimental data particularly in high compression region. Moreover, the present potential is also successful to give the third order elastic constants as well as first pressure derivative of second order elastic constants and isothermal bulk modulus. Phonon frequencies may also be calculated using the same potential which we will consider for future study.

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