

## **New General Equations for Calculation of Elements of Dynamical Matrix and Elastic Constants of BCC and FCC Metals**

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**Abstract:** *The generalized equations for calculation of elements of dynamical matrix and elastic constants of BCC and FCC metals are derived. These equations are expressed through radial and tangential force constants, which are derivations of the pair wise interatomic potential. The equations for elements of dynamical matrix are developed according to the de Launay method, and the equations for elastic constants are derived by using the Born-Begbie model. The suggested equations are alternative to widely used equations of G.L.Squires, which were expressed through the Born-von-Karman force constants. For verification of the equations, were calculated elastic constants of Li, K, Na, Rb, Cs, Al, Cu, Ag, and Pd within the frame of pseudopotential theory, which were found in satisfactory agreement with experimental data.*

**Keywords:** *dynamical matrix, radial and tangential force constants, elastic constants, pseudopotential theory*

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### **1. INTRODUCTION**

In calculations of the crystal lattice dynamics and elastic constants is still popular equations of G.L.Squires [1], which are expressed through the Born-von-Karman force constants. At first, the equations of G.L.Squires are successfully used by W.M.Shyu and G.D.Gaspari [2] for calculations of elastic constants of simple FCC and BCC metals within pseudopotential theory, but it was revealed that the theoretical values of Born-von-Karman force constants significantly differ from experimental values calculated from the fitting of experimental phonon spectra. In our opinion, Born-von-Karman force constants are not so convenient to use in fitting procedures of phonon spectra, because it is necessary up to six types of force constants on depending on the atomic coordinates.

A first-principles calculation of elastic constants of FCC metals and alloys within de Launay model [3] via the radial and tangential force constants on 10 nearest neighbor atoms is done by S.C. Upadhyaya et.al.[4,5]. They calculated elastic constants  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  of Ni, Pd, and alloys  $\text{Ni}_{0.55}\text{Pd}_{0.45}$ ,  $\text{Fe}_{0.92}\text{Co}_{0.08}$  with FCC crystal structure by applying the transition metal model potential of Animalu [6]. But formulas for calculation of the elastic constants  $C_{ij}$  and elements of dynamical matrix  $D_{ij}$  for FCC metals and alloys offered by S.C. Upadhyaya and his colleagues are not compact in comparison with expressions developed by G.L.Squires [1]. Portnoi K.I. et.al. [7] developed compact expressions for calculation of elastic constants  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  of BCC metals, but they managed to predict values only of  $C_{12}$  for K, Rb, and Cs. In our previous work [8,9] we calculated elastic constants  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  of alloys  $\text{Fe}_{0.975}\text{Rh}_{0.025}$  and  $\text{Fe}_{0.95}\text{Re}_{0.05}$  using expressions of [7] by applying the transition metal model potential of Animalu. The equations for calculation of elements of dynamical matrix and elastic constants of BCC metals were recently offered and successfully applied for calculation of elastic constants of alkali metals [10] also by authors of this work.

In the present work, the general equations for calculation of elastic constants  $C_{11}$ ,  $C_{12}$ ,  $C_{44}$  and elements of dynamical matrix  $D_{ij}$  of BCC and FCC metals via the radial and tangential force constants for arbitrary number of shells are developed within the de Launay model. For the verification of the offering equations, the elastic constants  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  of Li, Na, K, Rb, Cs, Al, Cu, Ag, Ni, and Pd are calculated using pseudopotentials and results are discussed in comparison with the existing experimental values and calculations of the other authors.

## 2. THEORY

According to [2], in case of central interaction, the first and second derivatives of pair potential  $V(r)$  provide for  $i^{\text{th}}$  set of neighbours the radial  $\alpha_i$  and tangential  $\beta_i$  force constants:

$$\alpha_i = [d^2V/dr^2]_{r_i}; \tag{1}$$

$$\beta_i = [(1/r) dV/dr]_{r_i}. \tag{2}$$

These force constants response for components of secular equation:

$$|D(\mathbf{q}) - 4\pi^2 M \nu^2 I| = 0, . \tag{3}$$

where  $D(\mathbf{q})$  is the dynamical matrix of order (3×3),  $I$  is the unit matrix,  $\nu$  is the normal mode phonon frequencies, and  $M$  is the ionic mass.

Within de Launay model [3] we wrote elements of dynamical matrix of secular equation (Eq. (3)) for FCC and BCC structures and generalized them to common expressions. Thus, the elements  $D_{ij}$  of symmetrical dynamical matrix  $D(\mathbf{q})$  are

$$D_{11} = \frac{1}{6} \sum_i N_i \{ \beta_i [6 - C_{h1}C_{k2}C_{l3} - C_{h1}C_{l2}C_{k3} - C_{k1}C_{h2}C_{l3} - C_{k1}C_{l2}C_{h3} - C_{l1}C_{h2}C_{k3} - C_{l1}C_{k2}C_{h3}] + \frac{(\alpha_i - \beta_i)}{h^2 + k^2 + l^2} [h^2(2 - C_{h1}C_{k2}C_{l3} - C_{h1}C_{l2}C_{k3}) + k^2(2 - C_{k1}C_{h2}C_{l3} - C_{k1}C_{l2}C_{h3}) + l^2(2 - C_{l1}C_{h2}C_{k3} - C_{l1}C_{k2}C_{h3})] \}; \tag{4}$$

$$D_{12} = \frac{1}{6} \sum_i N_i \frac{(\alpha_i - \beta_i)}{h^2 + k^2 + l^2} \{ hk(S_{h1}S_{k2}C_{l3} + S_{k1}S_{h2}C_{l3}) + hl(S_{h1}S_{l2}C_{k3} + S_{l1}S_{h2}C_{k3}) + kl(S_{k1}S_{l2}C_{h3} + S_{l1}S_{k2}C_{h3}) \}, \tag{5}$$

where  $i$  is number of shell,  $N_i$  is number of atoms on  $i^{\text{th}}$  shell,  $C_{hj} = \cos(haq_j/2)$ ,  $C_{kj} = \cos(kaq_j/2)$ ,  $C_{lj} = \cos(laq_j/2)$ ,  $S_{ij} = \sin(haq_j/2)$ ,  $S_{kj} = \sin(kaq_j/2)$ ,  $S_{lj} = \sin(laq_j/2)$ ,  $j=1,2,3$  ( $q_1 = q_x$ ;  $q_2 = q_y$ ;  $q_3 = q_z$ ), sets of  $(h,k,l)$  are coordinates of atoms in  $a/2$  unit,  $a$  is lattice parameter. Within the Born-Begbie model, from the elements of dynamical matrix  $D_{ij}$  (Eqs.(4)-(5)) in the long-wavelength limit of  $\mathbf{q} \rightarrow 0$  we obtained next expressions for the elastic constants of BCC and FCC metals:

$$C_{11} = \frac{1}{12a} \sum_i N_i \left\{ \beta_i (h^2 + k^2 + l^2) + [\alpha_i - \beta_i] \frac{h^4 + k^4 + l^4}{h^2 + k^2 + l^2} \right\}; \tag{6}$$

$$C_{44} = \frac{1}{12a} \sum_i N_i \left\{ \beta_i (h^2 + k^2 + l^2) [\alpha_i - \beta_i] \frac{h^2k^2 + h^2l^2 + k^2l^2}{h^2 + k^2 + l^2} \right\}; \tag{7}$$

$$C_{12} + C_{44} = \frac{1}{6a} \sum_i N_i [\alpha_i - \beta_i] \frac{h^2k^2 + h^2l^2 + k^2l^2}{h^2 + k^2 + l^2}. \tag{8}$$

(for the FCC metal values for  $C_{11}$ ,  $C_{12}$ ,  $C_{44}$  must be multiply by 2).

Pseudopotential theory in second order describes the interatomic interaction potential in the central pairwise form [2] like as:

$$V(r) = \frac{Z^2 e^2}{r} - \frac{2Z^2 e^2}{\pi} \int_0^\infty G(q) \frac{\sin(qr)}{qr} dq, \tag{9}$$

where  $Z$  is valence,  $e$  is electronic charge, and  $G(q)$  is the normalized energy wave-number characteristic given by:

$$G(q) = \left[ \frac{4\pi Z e^2}{\Omega_0 q^2} \right]^{-2} \frac{W^{bare}(q)^2}{1-f(q)} (1 - 1/\epsilon(q)). \tag{10}$$

$W^{bare}(q)$  is bare ion model potential and  $\varepsilon(q)$  is dielectric function according Hubbard [11] and Sham [12] and defined by

$$\varepsilon(q) = 1 + [1 - f(q)] \frac{4\pi Z e^{*2}}{\Omega_0 q^2} \left(\frac{2}{3} E_F\right)^{-1} \left[ \frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} \ln \left| \frac{2k_F + q}{2k_F - q} \right| \right],$$

where  $E_F = \frac{\hbar^2 k_F^2}{2m^*}$ ,  $k_F$  is the Fermi wave-number,  $m^*$  is effective mass of electron,

$$e^{*2} = (1 + \alpha_{eff})e^2, f(q) = \frac{q^2}{2(q^2 + k_F^2 + k_s^2)}, k_s^2 = \frac{2k_F}{\pi}.$$

The bare ion model potential form factor  $W^{bare}(q)$  depends on certain form of the model potential.

### 3. NUMERICAL RESULTS AND DISCUSSIONS

For verification of Eq. (6)-(8) we calculated elastic constants of some BCC alkali metals and FCC metals with comparison with experimental data and calculated results of other authors.

The radial  $\alpha_i$  and tangential  $\beta_i$  force constants of alkali metals Li, Na, K, Rb, and Cs are derived from the pair potential  $V(r)$ , which were calculated by using an analytic form for bare-ion pseudopotential form factor proposed by N.W.Ashcroft [13]. The Table I shows our calculated values of the tangential ( $\beta_i$ ) and radial force constants ( $\alpha_i$ ) for Na in comparison of results of [2], in which same model potential was used in calculations. Note that these results are sufficiently close.

**Table I.** Calculated values of the tangential ( $\beta_i$ ) and radial force constants ( $\alpha_i$ ) for Na in units  $10^{-3}$  N/m.

I	(hkl)	$N_i$	$\beta_i$		$\alpha_i$	
			ours	[2]	ours	[2]
1	111	8	-311.075	-310.61	4762.059	4764.66
2	200	6	72.463	72.47	943.846	940.68
3	220	12	7.411	7.41	-164.584	-163.24
4	311	24	-0.018	-0.14	20.736	20.48
5	222	8	1.006	0.82	21.849	22.39
6	400	6	1.249	1.17	-13.699	-13.68
7	331	24	-0.003	-0.11	-11.416	-11.23
8	420	24	-0.266	-0.34	-7.215	-7.00
9	422	24	-0.245	-0.30	5.057	5.25
10	333	8	0.079	0.04	4.616	4.62
	511	24	0.079	0.04	4.616	4.62
11	440	12	-0.165	-	5.086	-
12	531	48	0.156	-	-1.705	-

The Table II shows calculated elastic constants of Li, Na, K, Rb, and Cs. The elastic constants of Li are consistent with experimental values [14] and better than results of [15], which were calculated by using modified analytic embedded potential. Note that we calculated elastic constants of Li by using N.W.Ashcroft [13] potential with parameter of  $R_c = 1.284$ , which differs from parameter value chosen in [2], but our value is still in available range of parameter  $R_c$  [13]. Our results of calculation of elastic constants of Na, K, Rb, and Cs are satisfactory consistent with experimental data [16-19] and close to results [2], which calculated via Born-von-Karman force constants by using formulas of G.L.Squires [1]. In case of FCC metals we computed elastic constants of Al, Cu, Ag, Ni, and Pd (Table II). The elastic constants of Al calculated by using transition metal model potential of Animalu [6] are more close to experiment [20] than values of elastic constants calculated in [2] by using bare-ion pseudopotential of Ashcroft [13]. A success of computations of elastic constants depends on matching of model potential. Thus for Cu use of transition metal model potential of Animalu [6] is not reasonable, so it is hardly to achieve proper fitting of computational results to experimental data [21, 22] in this way. We attempted to apply the pseudopotential suggested by J.A.Moriarty[23] and managed to achieve a better consistence of calculations with experiment, which is shown in Table II. The results of calculation of elastic constants of Cu by the method of homogeneous deformation, using one-parameter model potential [24], gives value of  $C_{44}$  more close to the experiment than our calculated one.

However, transition metal model potential of Animalu [6] well suits for calculation of elastic constants of Ag, because our values of  $C_{11}, C_{12}$  are more close to experiment [21,22] than respective results of calculations carried out by using one-parameter model potential [24]. In cases of Ni and Pd, we improved a coincidence of calculations with experiment [25,26], although we used same model potential as in [4] and almost same set of force constants. Thus, Table III shows our calculated values of the tangential ( $\beta_i$ ) and radial ( $\alpha_i$ ) force constants for Ni, which are more close to the experiment than corresponding results of [4].

**Table II.** The elastic constants of pure metals in units  $10^{10} N/m^2$ .

Metal	Reference	$C_{11}$	$C_{12}$	$C_{44}$	Metal	Reference	$C_{11}$	$C_{12}$	$C_{44}$
Li	This paper	1.480	1.297	1.056	Al	This paper	11.483	3.080	3.545
	[15]	1.362	1.151	0.901		[2]	9.467	2.491	2.892
	Expt.(78K) [14]	1.486	1.274	1.048		Expt.(4.2K)[20]	11.43	6.19	3.16
Na	This paper	1.005	0.834	0.633	Cu	This paper	16.68	13.20	9.05
	[2]	1.008	0.842	0.637		[24]	16.105	11.821	7.700
	Expt.(78K) [16]	0.993	0.823	0.56		Expt.[21,22]	16.84	12.14	7.54
K	This paper	0.414	0.350	0.262	Ag	This paper	12.199	9.743	3.854
	[2]	0.413	0.345	0.268		[24]	11.824	10.210	4.989
	Expt.(4.2K)[17]	0.416	0.341	0.286		Expt.[21,22]	12.40	9.37	4.61
Rb	This paper	0.296	0.259	0.194	Ni	This paper	23.52	15.08	8.54
	[2]	0.283	0.235	0.190		[4]	22.78	17.84	8.70
	Expt. (80K)[18]	0.296	0.250	0.171		Expt.[25]	24.60	15.00	12.20
Cs	This paper	0.218	0.183	0.142	Pd	This paper	23.48	17.65	6.93
	[2]	0.221	0.185	0.143		[4]	24.37	17.57	8.55
	Expt.(78K)[19]	0.247	0.209	0.148		Expt.[26]	22.70	17.59	7.17

**Table III.** Calculated values of the tangential ( $\beta_i$ ) and radial force constants ( $\alpha_i$ ) for Ni in units  $10^{-3} N/m$ .

$i$	$(hkl)$	$N_i$	$\beta_i$		$\alpha_i$	
			ours	[4]	ours	[4]
1	110	12	-3441.55	-3503.39	41745.28	42076.75
2	200	6	-28.093	-28.15	303.213	292.92
3	211	24	94.919	95.25	31.002	60.23
4	220	12	9.909	10.82	-655.785	-652.32
5	310	24	-13.958	-14.28	185.985	182.69
6	222	8	8.612	8.27	151.771	160.37
7	321	48	5.741	6.00	-170.332	-167.57
8	400	6	-4.799	-4.64	-100.715	-91.96
9	330	12	-3.58	-3.75	105.671	97.87
	411	24	-3.58	-3.75	105.671	97.87
10	420	24	2.147	2.03	84.126	83.72
11	332	24	2.972	-	-40.107	-

#### 4. CONCLUSION

As shows existing experimental data and theoretical approaches, our expressions for calculation of elastic constants of Ni and Pd are more suitable than expressions developed in [4]. For Al, Cu, Ag, Ni, and Pd our expressions gives value of  $C_{11}$  in good agreement with experimental result, while one of the calculated values of  $C_{12}$  or  $C_{44}$  has considerable discrepancy with experimental data, and results of calculation depend on matching of model potential. In case of BCC alkali metals, our expressions are useful for evaluation of elastic constants.

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#### REFERENCES

- [1] G.L.Squires, Arkiv Fysik 25, 21(1963).
- [2] W.M.Shyu, G.D.Gaspari, Phys.Rev. 170, 687(1968).

- [3] De Launay. Solid State Physics. 2, 219(1956).
- [4] S.C.Upadhyaya, J.C Upadhyaya, R.Shyam, Phys.Rev. 44,122 (1991).
- [5] R.Shyam, S.C.Upadhyaya, J.C.Upadhyaya, Phys.Status Solidi B 161,565(1990).
- [6] A.O.E.Animalu, Phys.Rev.B8, 3542 (1973); Phys.Rev. B8,3555 (1973).
- [7] K.I.Portnoi, V.I.Bogdanov, D.L.Fuks, The calculation of interactions and the phase stability (Metallurgy, Moscow, 1981), p.248.
- [8] V.M.Silonov, L.Enkhtor, Izvestya vuzov 3, 71(1998).
- [9] V.M.Silonov, L.Enkhtor, Moscow University Phys. Bull. 3, 37(1997).
- [10] L.Ekhtor, V.M.Silonov, Bulletin of the Russian Academy of Sciences. Physics.78, 1163(2014).
- [11] J.Habbar, Proc. Roy. Soc.A 240, 539(1957); Proc. Roy. Soc. A 243,336(1958).
- [12] L.J.Sham, Proc. Roy. Soc. A 283, 33(1965).
- [13] N.W.Ashcroft, Phys. Letters 23, 48(1966); N.W.Ashcroft, and D.C.Langreth, Phys. Rev. 155, 682(1967).
- [14] H.C.Nash, C.S.Smith, J. Phys. Chem. Solids 9, 113(1959).
- [15] You Xie, Jiang-Min Zhang, Can.J.Phys. 86, 801(2008).
- [16] H.B.Huntington, Solid State Physics 7, 213(1958).
- [17] W.R.Marquart and J.Trivisonno, J. Phys. Chem. Solids 26, 273(1965).
- [18] E.J.Gutman, J.Trivisonno, J. Phys. Chem. Solids 28,805(1967).
- [19] F.J.Kollarits, J.Trivisonno, J. Phys. Chem. Solids 29, 2133(1968).
- [20] Kamm G.N., Alers G.A. J. Appl. Phys. 35, 327(1964).
- [21] B.Bacon, S.C.Smith, Acta metall. 4,337(1956).
- [22] E.Goens, J. Z.Weerts, Phys. 37,321(1936).
- [23] J.A. Moriarty Phys. Rev.B8,1639(1972).
- [24] F.A.Khwaja, M.S.K.Razmi, Phys. Status Solidi B 138,K95(1986).
- [25] J.A.Rayne, Phys. Rev. 118,1545(1960).
- [26] A.K.Ghatak, L.S.Kothari, Introduction to Lattice Dynamics (Addison Wesley, London,1972), p.234.