

Static and Vibrational Properties of Alkali Metals

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The computations of the static and vibrational properties of five alkali metals viz. Li, Na, K, Rb and Cs to second order in local model potential is discussed in terms of real-space sum of Born von Karman central force constants. The exchange and correlation functions due to Hartree (H) and Ichimaru-Utsumi (IU) are used to investigate influence of screening effects. Results for the lattice constants i.e. C_{11} , C_{12} , C_{44} , $C_{12} - C_{44}$, C_{12}/C_{44} and bulk modulus B obtained using the Hartree (H) local field correction function has higher values in comparison with the results obtained for the same properties using Ichimaru-Utsumi (IU) local field correction function. The results for the Shear modulus (C'), deviation from Cauchy's relation, Poisson's ratio σ , Young modulus Y , propagation velocity of elastic waves, phonon dispersion curves (PDC) and degree of anisotropy A are highly appreciable for the alkali metals. The phonon frequencies of alkali metals in the longitudinal branch are more sensitive to the exchange and correlation effects in comparison with the transverse branches. The phonon dispersion curves (PDC) of pure alkalis are found in qualitative agreement with the available experimental data. While, the frequencies in the longitudinal branch are suppressed due to IU-screening function than the frequencies due to static H-screening function.

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1. Introduction

In the study of various properties of solids, one frequently requires the knowledge of interaction energy between the ions or atoms. The studies of a pair effective interionic interaction in simple metals has yet a long history and originally they were not systematized and were concerned with individual metals groups of metals. In recent years considerable attention has been devoted to the theoretical study of the nature of effective interaction between constituent atom or ion in simple metals [1-5]. The analysis of such studies allows us to conclude : (1) this interaction in metals arises due to interatomic spacing in metals, (2) the potential energy of an effective pair interaction has sufficiently deep minima in a negative energy region, (3) the depth of a potential well increases with increase of a valence and (4) the interatomic distance, corresponding to the potential energy minimum, increases with the increase of an atomic

number. The knowledge of interatomic potential is very essential for determining various static and vibrational properties of materials. The atoms in the metals and alloys are attached with one another, elastically. The pair potential provides a way to look into the nature of binding forces between the atoms in a matter.

The pseudopotential approach is proved one of the best methods in computing the

pair potentials, but the studies on the pair potential of metallic elements and related properties are not yet taken up, systematically. There are some attempts on the investigation of static and vibrational properties of bcc alkali metals and their alloys based on pseudopotential theory [1-6]. But studies on simple systems of bcc alkali metals and their alloys are not rigorous enough, especially the computations of elastic constants, bulk modulus and phonon dispersion relations [1-6]. Therefore,

we have decided to work on alkali metals viz. Li, Na, K, Rb and Cs. In the present article, the real space sum analysis [1-6] is used to compute phonon dispersion relation along three major symmetry directions. Very recently, we have reported static and vibrational properties of equiatomic Na-based binary alloys [3] using model potential formalism. Well known empty core (EMC) model potential of Ashcroft [7] is used to describe the electron-ion interaction for alkali systems. For the first time an advanced and more recent local field correlation function due to Ichimaru-Utsumi (IU) [8] has been employed in such investigations. This helps in identifying the influence of exchange and correlation effects in the static form of Hartree (H) (only static) dielectric function [9].

II. Theoretical Methodology

The phonon frequencies can be obtained by solving the standard secular determinantal equation [1-3]

$$\det[D_{\alpha\beta}(q) - 4\pi^2\nu^2 M \delta_{\alpha\beta}] = 0, \quad (1)$$

where, M is the ionic mass, ν is the phonon frequency and $D_{\alpha\beta}(q)$ is the dynamical matrix in which the force between two ions depends only upon the distance between them is given by,

$$D_{\alpha\beta}(q) = \sum_n (1 - e^{i\mathbf{q}\cdot\mathbf{r}}) \left. \frac{d^2\Phi(r)}{dr_\alpha dr_\beta} \right|_{r=r_n}, \quad (2)$$

here $\Phi(r)$ is the interionic pair potential, r_α and r_β are the α^{th} and β^{th} Cartesian components of the position vector of n^{th} ion, respectively.

This dynamical matrix element used in the present calculation finally takes the form,

$$D_{\alpha\beta}(q) = \sum_n (1 - e^{i\mathbf{q}\cdot\mathbf{r}}) \left[K_t + \frac{r_\alpha r_\beta}{r^2} (K_r - K_t) \right], \quad (3)$$

Here K_t and K_r are the force constants between a pair of ions interacting through a central interaction and n specifies shell index.

$$K_t = \frac{1}{r} \frac{d\Phi(r)}{dr} = -\frac{Z^2 e^2}{r^3} + \frac{\Omega_0}{\pi^2 r^2} \int_0^\infty F(q) q^2 \left[\cos(qr) - \frac{\sin(qr)}{qr} \right] dq. \quad (4)$$

$$K_r = \frac{d^2\Phi}{dr^2} = \frac{2Ze^2}{r^3} + \frac{\Omega_0}{\pi^2 r^2} \int_0^\infty F(q) q^2 \left[\frac{2\sin(qr)}{qr} - 2\cos(qr) - qr\sin(qr) \right] dq. \quad (5)$$

Where $F(q)$ is the energy wave number characteristic given by

$$F(q) = \frac{\Omega_0 q^2}{8\pi e^2} |W_B(q)|^2 \frac{[\varepsilon_H(q) - 1]}{1 + [\varepsilon_H(q) - 1][1 - f(q)]}. \quad (6)$$

With Ω_0 , $W_B(q)$, $\varepsilon_H(q)$ and $f(q)$ are the atomic volume, bare-ion pseudopotential, static Hartree dielectric function [7] and local field correlation function, respectively.

The bare-ion empty core (EMC) model potential of Ashcroft [7] is given by

$$V(q) = \frac{-8\pi Z}{\Omega_0 q^2} \cos(qr_c). \quad (7)$$

here, Z , Ω_0 and r_c are the valence, atomic volume and parameter of the model potential, respectively.

Using these atomic force constants, we can generate inter atomic force constants $K_{\alpha\beta}$ which can then be employed to investigate the elastic constants

$$K_{\alpha\beta} = \frac{d^2\Phi(r)}{dr_\alpha dr_\beta} = \left[\delta_{\alpha\beta} - \frac{r_\alpha r_\beta}{r^2} \right] K_t + \frac{r_\alpha r_\beta}{r^2} K_r. \quad (8)$$

Under the long wave phonon method, the elastic constants are studied by [1-3]

$$C_{11} = \frac{1}{12a} \sum_n N(n) [x^2 K_{xx}^n + y^2 K_{yy}^n + z^2 K_{zz}^n], \quad (9)$$

$$C_{44} = \frac{1}{24a} \sum_n N(n) [(y^2 + z^2) K_{xx}^n + (z^2 + x^2) K_{yy}^n + (x^2 + y^2) K_{zz}^n], \quad (10)$$

$$C_{12} + C_{44} = \frac{1}{6a} \sum_n N(n) [yz K_{yz}^n + zx K_{zx}^n + xy K_{xy}^n]. \quad (11)$$

Where “ a ” is the lattice constant and $N(n)$ is the number of atoms at the n^{th} neighbour separation.

The shear modulus C' and bulk modulus B are given by [1-3]

$$C' = \left[\left(\frac{C_{11} - C_{12}}{2} \right) \right]. \quad (12)$$

and

$$B = \left[\frac{(C_{11} + 2C_{12})}{3} \right]. \quad (13)$$

The extent to which the interatomic forces are non-pair wise can be obtained by investigating the breakdown of the Cauchy relation. The Cauchy's ratio is obtained by C_{12}/C_{44} .

Poisson's ratio σ is second independent elastic parameter determined as [1-3],

$$\sigma = \frac{C_{12}}{(C_{11} + C_{12})}. \quad (14)$$

From the calculated values of the bulk modulus and Poisson's ratio, Young modulus Y is derived as [1-3],

$$Y = 3B(1 - 2\sigma). \quad (15)$$

In the cubic system the propagation velocity of longitudinal and transverse waves in [100], [110] and [111] directions are given as [1-3]

$$v_L[100] = \left[\frac{C_{11}}{\rho} \right]^{1/2}. \quad (16)$$

$$v_L[110] = \left[\frac{(C_{11} + C_{12} + 2C_{44})}{2\rho} \right]^{1/2}. \quad (17)$$

$$v_L[111] = \left[\frac{(C_{11} + 2C_{12} + 4C_{44})}{3\rho} \right]^{1/2}. \quad (18)$$

$$v_T[100] = v_{T1}[110] = \left[\frac{C_{44}}{\rho} \right]^{1/2}. \quad (19)$$

$$v_{T2}[110] = \left[\frac{(C_{11} - C_{12})}{2\rho} \right]^{1/2}. \quad (20)$$

$$v_T[111] = \left[\frac{(C_{11} - C_{12} + 2C_{44})}{3\rho} \right]^{1/2}. \quad (21)$$

The behavior of phonon frequencies in the limit independent of direction is given by [1-3]

$$Y_1 = \lim_{q \rightarrow 0} \sum_i \frac{\omega_i^2(q)}{q^2} = \left[\frac{(C_{11} + 2C_{44})}{\rho} \right], \quad (22)$$

and

$$Y_2 = \lim_{q \rightarrow 0} \left(\frac{\omega_{T1}}{\omega_{T2}} \right)^2 = \left[\frac{(C_{11} - C_{12})}{2C_{44}} \right]. \quad (23)$$

The degree of elastic anisotropy A is the inverse of Y_2 , i.e. [1-3],

$$A = \left[\frac{2C_{44}}{(C_{11} - C_{12})} \right]. \quad (24)$$

The value of A is unity when the material is elastically isotropic and differs from unity otherwise.

In evaluating integration in Eqs. (4) and (5), the upper limit of integral is taken $40 k_F$ so that, a complete convergence of the model potential is achieved at higher momentum transfer and it covers all the oscillations of the form factor. Therefore, any artificial/fictitious cut-off in the present computations is avoided. We have performed the real space sum analysis up to 33 sets of nearest neighbours in r -space, which are found sufficient for computing the elastic constants and bulk modulus using interatomic force constants, to consider a long-range character for proper convergence of the calculation and to achieve desired accuracy.

III. Results and discussion

The input parameters viz. Z , Ω_O , k_F and r_C used in the present computations of the static and vibrational properties of alkali metals are taken from [11].

In the present computation, the bcc crystal structure considered for all alkali metals. The lattice constants ' a ' are obtained from the well known relation $(2\Omega_O)^{1/3}$. Tables 1-7 display the computed values of some static and vibrational properties of alkali metals. It is noted from the Tables 1-7 that, our results calculated for C_{11} , C_{12} , C_{44} , $C_{12} - C_{44}$, C_{12}/C_{44} and bulk modulus B from H-local field correction function give higher values than those obtained for the IU-local field correction functions. There is a good agreement for the calculated values of the Shear modulus C' , deviation from Cauchy's relation, Poisson's ratio σ , Young modulus Y , propagation velocity of elastic waves, phonon dispersion curves (PDC) and degree of anisotropy A using H and IU-local field correction functions.

The present results are compared with the experimentally [11] and theoretically [12-25] available data and found in qualitative agreement with them. It is noticed from the present study that, the percentile influence of the IU-local field correction function with respect to the static H-local field correction function on the vibrational properties of Li, Na, K, Rb and Cs is found 0.82%-76.59%, 0.59%-40.99%, 2.12%-62.58%, 3.72%-52.74% and 3.23%-36.41%, respectively. This clearly indicates that the local field correlations play a very effective role in explaining correctly the static and dynamic properties of such solid solutions. The calculated results of the vibrational properties of Li, Na, K, Rb and Cs alkali metals deviate in the range of 6.55%-985.68%, 2.06%-1900.12%, 0.26%-454.59%, 0.28%-868.06% and 0.45%-680.79% from the highest experimental findings [11], respectively. The present results of the vibrational properties are found in qualitative agreement with the other such available experimental [11] and theoretical [12-25] data

The phonon dispersion curves (PDC) of five alkali metals viz. Li, Na, K, Rb and Cs along [100], [110] and [111] directions of high symmetry, which are shown in Figures 1-5 with available experimental findings [26-29]. The present results of pure alkali elements are found in qualitative agreement with the experimental data [26-29]. We have found that the phonon frequencies in the longitudinal branch are more sensitive to the exchange and correlation effects in comparison with the transverse branches. The frequencies in the longitudinal branch are suppressed due to IU-screening function than the frequencies due to static H-screening function. While in the transverse branch effect of exchange and correlation enhances slightly the phonon modes. It is found that at the zone boundaries of [100] and [111] directions, i.e., for the larger momentum transfer the effect of local field correlation is almost negligible. These dispersion curves are not showing any abnormality in the three regions of high symmetry directions and exhibiting qualitative behaviour.

From the Figures 1-5, we observe that, when we move from Li \rightarrow Cs, the phonon frequency decreases with increase in the average volume of the metallic

elements. The phonon dispersion curves (PDC) are seen to be quite unsatisfactory except near the small k -regions ($k < 0.6$ or so) because of the uncertainty of the experimental data of the pure metallic elements. For Rb and Cs, present results deviate more from the experimental points. The comparisons between present data and experimental findings favour and confirm. Also, in the absence of experimental information such calculations may be considered as one of the guidelines for further investigations either theoretical or experimental. Hence, such study could be extended for the other types of the metals.

VI. Conclusions

At the end, we conclude that the presently computed results of the static and vibrational properties of pure alkali elements are found in qualitative agreement with the experimental and theoretical data. From the present experience, we also conclude that it should be interesting to apply other local pseudopotentials for such comprehensive study to judge and confirm the wider applicability of the potential.

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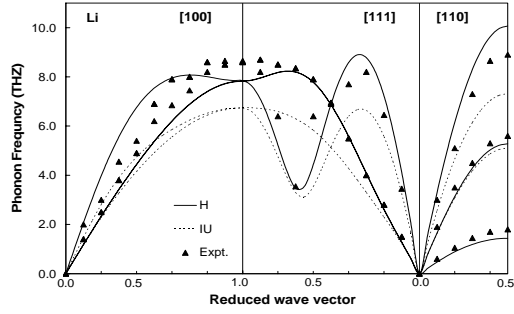


Fig. 1. Phonon dispersion curves of Li.

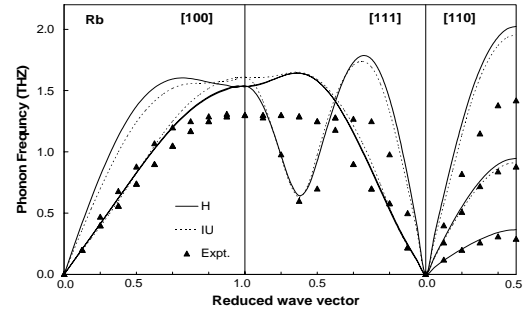


Fig. 4. Phonon dispersion curves of Rb.

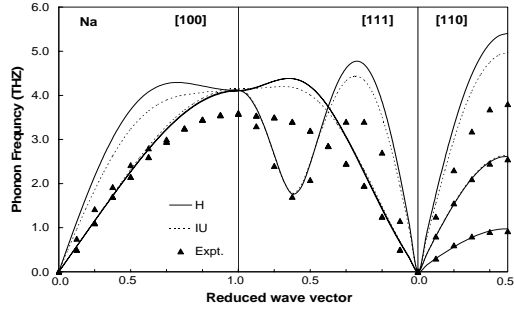


Fig. 2. Phonon dispersion curves of Na.

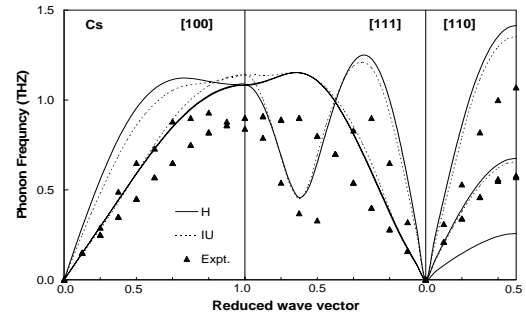


Fig. 5. Phonon dispersion curves of Cs.

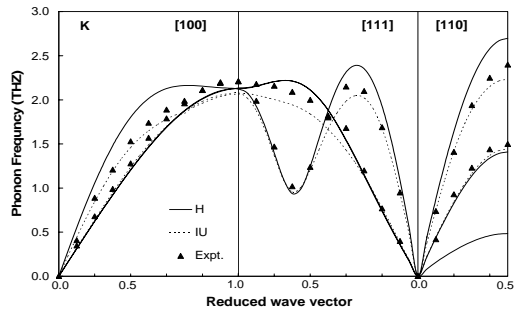


Fig. 3. Phonon dispersion curves of K.

Table 1. Dynamical elastic constants (in 10^{11} dyne/cm²) for Li.

Prop.	Present results		Expt. [11]	Others [12-25]
	H	IU		
C₁₁	2.9026	1.4462	1.571	1.51, 2.023, 1.62, 1.84, 1.77, 3.762, 1.543, 1.570, 2.050, 1.437, 6.000, 1.68, 1.57, 1.472, 2.361, 1.539, 1.532, 1.40, 1.712, 4.465, 4.83, 1.388, 1.567, 2.072, 1.610, 1.530, 1.548
C₁₂	2.7686	1.3481	1.329	1.274, 1.877, 1.44, 3.401, 1.173, 1.379, 1.284, 1.29, 3.395, 1.293, 1.39, 1.43, 1.853, 1.555, 1.274, 1.272, 1.57, 1.982, 1.556, 1.40, 4.070, 1.212, 1.283, 1.291, 1.279, 1.59, 1.639
C₄₄	0.9338	0.9185	1.16	1.050, 0.937, 1.07, 1.336, 7.794, 1.390, 1.15, 0.904, 2.654, 1.079, 1.11, 1.08, 1.257, 1.371, 1.106, 1.17, 1.22, 1.128, 1.115, 1.10, 1.233, 1.191, 1.380, 1.053, 1.231, 1.544
C'	0.0670	0.0490	0.121	1.118, 0.703, 1.20, 0.072, 0.089, 0.77, 0.532
B	2.8133	1.3808	1.410	1.353, 1.926, 3.756, 1.349, 2.1081, 3.71, 1.183, 1.324, 1.341, 1.917, 1.248, 1.442, 1.783, 1.262, 1.297, 1.608, 1.246, 1.626, 3.517, 1.373, 1.246

Table 2. Dynamical elastic constants (in 10^{11} dyne/cm²) for Na.

Prop.	Present results		Expt. [11]	Others [12-25]
	H	IU		
C₁₁	2.3897	1.7361	0.893, 0.857, 0.85	1.049, 1.201, 0.98, 0.810, .0168, 1.064, 0.808, 0.816, 0.814, 0.866, 1.020, 0.116, 0.891, 1.069, 0.821, 0.910, 0.740, 0.792, 0.786, 0.912, 1.657, 1.220, 1.260, 0.924, 1.100, 1.014, 0.616, 1.010, 0.810, 0.832, 0.546, 0.958, 1.120, 1.280
C₁₂	2.2264	1.5695	0.738, 0.711, 0.704	0.894, 1.001, 0.860, 0.644, 0.059, 0.742, 0.420, 0.799, 0.827, 0.990, 1.070, 1.044, 0.737, 0.873, 0.686, 0.740, 0.630, 0.693, 0.688, 0.705, 0.672, 0.850, 0.830, 0.955, 0.838, 0.910, 0.085, 0.475, 0.692, 0.789, 1.502, 0.777, 0.683, 1.050, 0.880
C₄₄	0.6062	0.6134	0.66,	0.594, 0.529, 0.590, 0.690, 0.520, 0.711, 0.550, 0.663, 0.735, 0.573,

			0.63, 0.588	0.587, 0.553, 0.66, 0.595, 0.654, 0.580, 0.068, 0.680, 0.067, 0.775, 0.539, 0.579, 0.630, 0.055, 0.028, 0.610, 0.064, 0.068, 0.067, 0.549, 0.558
C'	0.0802	0.0833	0.077, 0.073	0.077, 0.100, 0.081, 0.077, 0.098, 0.043, 0.083
B	2.2798	1.6250	0.79, 0.76	0.946, 1.068, 0.699, 0.736, 0.730, 0.760, 0.718, 0.746, 0.742, 0.788, 0.938, 0.728, 0.830, 1.554, 0.807, 0.699, 0.743, 1.009, 0.866, 0.903, 0.773, 0.474, 0.851, 0.794, 0.766, 0.753, 0.722

Table 3. Dynamical elastic constants (in 10^{11} dyne/cm²) for K.

Prop.	Present results		Expt. [11]	Others [12-25]
	H	IU		
C₁₁	0.7582	0.5088	0.416	0.499, 0.555, 0.410, 0.399, 0.420, 0.510, 0.402, 0.425, 0.304, 0.495, 0.530, 0.434, 0.481, 0.421, 0.50, 0.592, 0.616, 0.409, 0.395, 0.327, 0.480, 0.530, 0.503, 0.450, 0.478, 0.390, 0.565, 0.384, 0.394, 0.482, 0.466, 0.460
C₁₂	0.7175	0.4331	0.341	0.441, 0.465, 0.35, 0.322, 0.35, 0.406, 0.332, 0.381, 0.240, 0.429, 0.44, 0.360, 0.415, 0.344, 0.41, 0.541, 0.491, 0.346, 0.324, 0.327, 0.42, 0.439, 0.37, 0.401, 0.34, 0.519, 0.325, 0.035, 0.411, 0.410, 0.10
C₄₄	0.2461	0.2567	0.286	0.254, 0.259, 0.26, 0.34, 0.256, 0.263, 0.253, 0.29, 0.26, 0.251, 0.260, 0.288, 0.346, 0.269, 0.276, 0.28, 0.29, 0.264, 0.255, 0.27, 0.286, 0.359, 0.272, 0.269, 0.29, 0.25, 0.259
C'	0.0325	0.0379	0.038	0.029, 0.045, 0.023, 0.037, 0.033, 0.032, 0.038
B	0.7392	0.4583	0.366	0.460, 0.495, 0.106, 0.263, 0.451, 0.358, 0.368, 0.315, 0.534, 0.385, 0.437, 0.349, 0.349, 0.385, 0.348, 0.378, 0.427, 0.460, 0.366, 0.435, 0.424, 0.395, 0.376, 0.366, 0.348

Table 4. Dynamical elastic constants (in 10^{11} dyne/cm²) for Rb.

Prop.	Present results		Expt. [11]	Others [12-25]
	H	IU		

C₁₁	0.9292	0.6861	0.316, 0.342	0.333, 0.311, 0.332, 0.42, 0.372, 0.35, 0.33, 0.453, 0.379, 0.33, 0.305, 0.431, 0.318, 0.31, 0.29, 0.445, 0.410, 0.31, 0.318, 0.518, 0.322, 0.38, 0.30
C₁₂	0.8692	0.6497	0.257, 0.288	0.267, 0.273, 0.271, 0.34, 0.319, 0.30, 0.28, 0.420, 0.355, 0.27, 0.256, 0.34, 0.263, 0.26, 0.24, 0.413, 0.33, 0.26, 0.269, 0.415, 0.263, 0.31, 0.25
C₄₄	0.2206	0.2045	0.211, 0.221	0.193, 0.195, 0.220, 0.278, 0.207, 0.20, 0.19, 0.285, 0.20, 0.172, 0.198, 0.20, 0.197, 0.279, 0.209, 0.22, 0.19, 0.278, 0.22, 0.173, 0.200, 0.20, 0.27, 0.240, 0.21, 0.20, 0.172, 0.21, 0.20
C'	0.0300	0.0182	0.030, 0.027	0.020, 0.037, 0.016, 0.024, 0.038, 0.012, 0.026
B	0.8892	0.6618	0.277, 0.306	0.289, 0.264, 0.322, 0.261, 0.285, 0.311, 0.272, 0.363, 0.290, 0.283, 0.424, 0.306, 0.285, 0.359, 0.282, 0.285

Table 5. Dynamical elastic constants (in 10^{11} dyne/cm²) for Cs.

Prop.	Present results		Expt. [11]	Others [12-25]
	H	IU		
C₁₁	0.6423	0.4667	0.260	0.282, 0.23, 0.235, 0.27, 0.26, 0.351, 0.306, 0.22, 0.271, 0.24, 0.21, 0.365, 0.239, 0.258, 0.16, 0.28, 0.22
C₁₂	0.5990	0.4392	0.216	0.264, 0.19, 0.196, 0.23, 0.22, 0.235, 0.232, 0.22, 0.232, 0.20, 0.17, 0.327, 0.209, 0.290, 0.099, 0.24, 0.18
C₄₄	0.1617	0.1514	0.160	0.146, 0.144, 0.166, 0.15, 0.13, 0.13, 0.147, 0.15, 0.146, 0.16, 0.14, 0.144, 0.14, 0.16, 0.15, 0.124
C'	0.0217	0.0138	0.022	0.009, 0.019, 0.037, 0.019, 0.015
B	0.6135	0.4483	0.231	0.270, 0.209, 0.340, 0.239, 0.213, 0.257, 0.245, 0.266, 0.245, 0.243, 0.219, 0.2174, 0.282, 0.217

Table 6. Deviation from Cauchy relation (10^{11} dynes/cm²), Cauchy's ratio, Poisson ratio and Young's modulus (10^{11} dynes/cm²), Degree of anisotropy, phonon frequencies limit for alkali metals.

Prop.	Present results		Expt. [3.30, 3.31]	Others
	H	IU		
Li				
C ₁₂ -C ₄₄	1.8348	0.4296	0.1690	—
C ₁₂ /C ₄₄	2.9648	1.4678	1.1456, 1.3000	3.43
σ	0.4882	0.4825	0.4582	—
Y	0.1994	0.1454	3.5290	—
A	13.9355	18.7296	—	—
y1	8.8839	6.1142	—	—
y2	0.0718	0.0534	—	—
Na				
C ₁₂ -C ₄₄	1.6201	0.9560	0.0810, 0.0780	—
C ₁₂ /C ₄₄	3.6734	2.5584	1.4800, 1.1181, 1.1285	3.05
σ	0.4826	0.4748	0.4524, 0.4534, 0.4300	0.49
Y	0.2377	0.2457	2.2520, 2.1220	—
A	7.5618	7.3672	—	—
y1	3.5544	2.9261	—	—
y2	0.1322	0.1358	—	—
K				
C ₁₂ -C ₄₄	0.4714	0.1764	0.0850	—
C ₁₂ /C ₄₄	2.9152	1.6872	1.1923, 1.6700	2.72
σ	0.4783	0.4598	0.4504	—
Y	0.0960	0.1106	1.087	—
A	7.5787	6.7739	—	—
y1	1.4001	1.1228	—	—
y2	0.1319	0.1476	—	—
Rb				
C ₁₂ -C ₄₄	0.6486	0.4451	0.067, 0.046	—
C ₁₂ /C ₄₄	3.9395	3.1764	1.2180, 1.3031	—
σ	0.4833	0.4864	0.4485, 0.4571	—
Y	0.0890	0.0541	0.8555, 0.7868	—
A	7.3534	11.2317	—	—
y1	0.8410	0.6720	—	—
y2	0.1360	0.0890	—	—
Cs				
C ₁₂ -C ₄₄	0.4373	0.2878	0.0560	—
C ₁₂ /C ₄₄	3.7041	2.9000	1.3500	—
σ	0.4826	0.4848	0.4567	—
Y	0.0642	0.0409	0.6405	—
A	7.4703	11.0032	—	—
y1	0.4833	0.3851	—	—
y2	0.1339	0.0909	—	—

Table 7. Propagation velocities (10^5 cm/sec) of elastic waves in alkali metals

Prop.	Present results		Expt. [11]
	H	IU	
Li			
V _L (100)	7.3524	5.1897	5.3907
V _T (100)	4.1702	4.1358	4.6322
V _L (110)	8.3786	6.5669	6.9483
V _{Ti} (110)	4.1702	4.1358	4.6322
V _{T2} (110)	1.1171	0.9556	1.4960
V _L (111)	8.6937	6.9657	7.3950
V _T (111)	2.5747	2.5121	2.9401
Na			
V _L (100)	4.8549	4.1406	2.9594, 2.8991
V _T (100)	2.4468	2.4613	2.5442, 2.4857
V _L (110)	5.3633	4.7308	3.8041, 3.7240
V _{Ti} (110)	2.4468	2.4613	2.9594, 2.8991
V _{T2} (110)	0.8898	0.9071	0.8718, 0.8461
V _L (111)	5.5224	4.9117	4.0466, 3.9609
V _T (111)	1.5886	1.6024	1.6323, 1.5927
K			
V _L (100)	2.9316	2.3641	2.1301
V _T (100)	1.6442	1.6791	1.7602
V _L (110)	3.3077	2.8270	2.6922
V _{Ti} (110)	1.6442	1.6791	1.7662
V _{T2} (110)	0.5973	0.6451	0.6395
V _L (111)	3.4239	2.9653	2.8550
V _T (111)	1.0672	1.1033	1.1456
Rb			
V _L (100)	2.3879	2.0519	1.3876, 1.4436
V _T (100)	1.1636	1.1203	1.1339, 1.1604
V _L (110)	2.6214	2.3138	1.7411, 1.8072
V _{Ti} (110)	1.1636	1.1203	1.1339, 1.1604
V _{T2} (110)	0.4291	0.3343	0.4239, 0.4056
V _L (111)	2.6948	2.3947	1.8440, 1.9132
V _T (111)	0.7577	0.7020	0.7405, 0.7336
Cs			
V _L (100)	1.7928	1.5282	1.1366
V _T (100)	0.8996	0.8705	0.8916
V _L (110)	1.9784	1.7391	1.4063
V _{Ti} (110)	0.8996	0.8705	0.8916
V _{T2} (110)	0.3291	0.2624	0.3306
V _L (111)	2.0368	1.8039	1.4853