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Theoretical investigation on the structural and vibrational properties of some alkali liquid metals: A pseudopotential approach

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Abstract

Along with a few elastic constants, a recently created pseudopotential is employed to examine the vibrational properties of some simple alkali metals, i.e. Li, Na, K, Rb and Cs. The phonon dispersion curves (PDC) are computed in the text. (ω_L *and* ω_T), *longitudinal sound velocity* (v_l), *transverse sound velocity* (v_t), *isothermal bulk modulus* (B), *modulus of rigidity* (G), *Young's modulus* (Y), *Debye temperature* (θ_D) *of some liquid alkali metals. The second order technique used in the current work, using Hubbard and Beeby (HB) equations, is based on pseudopotential theory. The various Percus-Yevick hard sphere (PYHS) and one-component plasma (OCP) structure factors used in the current investigation are used to construct the pair correlation function* $g(r)$. *The current paper makes use of three distinct forms of local field correction functions developed by Hartree (H), Taylor (T), and Nagy (N). The current findings are found to qualitatively agree with the experimental and theoretical data that is currently available.*

Keywords
Pseudopotential; Liquid metals, PYHS structure factor, OCP structure factor, phonon dispersion, structural properties, vibrational properties.

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1 Introduction

Since a long time, phonon dispersions and vibrational properties in liquids and gases have been explored theoretically, through computer simulation, and empirically. The most popular and useful experimental technique for determining phonon dispersion curves is neutron scattering. Neutron scattering research has supplied some basic excitation in liquid metals. From Copley and et al. [1] to Cabrillo et al. [2,3], the key experimental work sheds information on the dynamical features of alkali metals. Desai et al. [4] theoretically reported the vibrational characteristics of liquid argon before this practical investigation.

Theoretically, phonon dispersion curves can be obtained using force constants, however even for regular and simple systems such as cubic crystals, the number of force constants required is large. As a result, for complicated systems such as liquids, phonon models that represent the ion-electron interaction are critical [5]. So, since liquid metal is a highly correlated system, the random phase approximation cannot produce an accurate picture of interaction. however, Hubbard and Beeby (HB) [6] has explained the vibrational properties of liquid metals quite effectively, and it may also be called a generalization of theory for the solid up to the liquid state. For the explanation of phonon in liquid metals, a stepwise generalized phonon theory of the crystal has been made. In the first solid state, there is no relative motion expected but in the other half, it is to be extended to the continuous system with the relative atomic motion which is called the liquid metals. To take the work based on the theoretical formulation, the high degree physics needed which includes the kinetics with the coupling of various modes [7,8]. These excitations are density dependent functions so, they follow, in some manner, the structure factor variations with respect to wave numbers. The structure factor peak position falls roughly at the minima of the longitudinal frequency ω_L vs. wave vector (k) plot [9].

Numerous studies on the vibrational characteristics of numerous types of materials have been published [10–12]. Thakor and his colleagues [12] used the HB method to calculate phonon dispersion curves. The same calculations were made for the metallic elements such as Na, Mg, Al and Pb. The acquired values in that study are consistent with the experimental data for Na elements. Since there are just a limited amount of experimental data points available for Al, it was not displayed. Vora [11] has published the phonon dispersion curves for liquid alkali metals after around a year. With the aid of the empty core model pseudopotential, he demonstrated how the curves are behaving consistently. The comparison with the experimental data available reveals that the selection of potential may be to blame for the low agreement. Recently, Malan and Vora [12] have made another attempt to determine the PDC of liquid alkali metals. They claimed that the HB technique can be used to measure the material's aforementioned attribute. The curves they obtained were found to be compatible with the experimental data that was available [12].

Looking to the advantages of pseudopotential theory with HB approach particularly for studying the vibrational properties of studied simple liquid alkali metals are reported in the present article. For studying the vibrational properties, the structure factor S(q) and then after pair correlation function g(r) plays an important role. Therefore, our motive of the present article is studying the vibrational properties of some simple liquid metals with Percus-Yevick hard sphere (PYHS) [13–15] and one-component plasma (OCP) [16–18] structure factor models with our own developed single parametric model pseudopotential.

2 Computational Methodology

The size and locations of the longitudinal (L) and transverse (T) frequency peak positions with respect to the wave vector k are attempted to be determined in the current article. In the current investigation, the pseudopotential concept was used. The determined values of the pseudopotential parameter were applied to the newly constructed pseudopotential. When calculating the ion-interaction, the exchange and correlation effects must also be taken into consideration. To have the highest chance of predicting the astonishing results, the most appropriate exchange and correlation functions are advised.

Here we are using two different methods for the calculation of structure factor, i.e., PYHS [13–15] and OCP [16–18]. To obtain the structure factor by OCP method, we require a pseudopotential. For the same reason, we have applied our own generated model pseudopotential to obtain the pair distribution function with the help of which we will calculate the vibrational properties of the liquid alkali metals.

The form of our newly proposed model potential in real space and corresponding bare-ion form factor in the reciprocal space is given as

$$\begin{aligned} V(r) &= \frac{-3Ze^2}{r} + \frac{Ze^2}{r} exp\left(1 - \frac{r}{r_c}\right) \quad r \le r_c \\ &= -\frac{Ze^2}{r} \quad r \ge r_c \end{aligned} \tag{1}$$

The Fourier transform of such model potential is given as

$$\begin{aligned} V(q) = -\frac{4\pi Ze^2}{q^2\Omega_0}[3 - \frac{q^2r_c^2}{1+q^2r_c^2} - exp(1) + \{-2 + exp(1) \\ + \frac{exp(-1)q^2r_c^2}{1+q^2r_c^2}\}\cos qr_c + \frac{exp(-1)qr_c}{1+qr_c^2}\sin qr_c] \end{aligned} \tag{2}$$

Here, Z and e are valency and electronic charge, Ω_0 is atomic volume, q is wave vector, and r_c is the parameter of the potential, respectively. It should be noticed that this type of pseudopotential only has one parameter r_c. Within the core region, it is continuous at $r = r_c$ and becomes weaker and weaker as r decreases. Two features of this form are the Coulombic terms inside the core and the fluctuating cancellation brought on by the attracting and repelling concentrations of the potential outside the core. It is thought that instead of being 0 or constant, the potential outside the core should change as a function of r. This demonstrates the modification made to the Ashcroft empty core model. The pseudopotential parameter d can be identified using [19] as

$$r_c = 0.51 R_a Z^{-1/3} \tag{3}$$

The pair correlation function g(r) and the pair potential must be obtained in order to carry out the computations. This method generates pair correlation function values as a prerequisite for subsequent calculations rather than directly extracting them from the experimental data. Therefore, the current prediction is entirely theoretical and has no connection to any earlier experimental studies. By using the generated S(q) from the PYHS [13-15] and OCP [16-18] the g(r) par distribution function for the respective reference system can be easily obtained. Here [20] is an equation for the g(r) utilized in this calculation.

$$g(r) = 1 + \left(\frac{1}{2\pi^2 \rho r}\right) \int_0^\infty q[S(q) - 1]\sin(qr)dq \tag{4}$$

The structure factor equations of PYHS [13–15] can be derived as:

$$\begin{aligned} S(q) = [1 + \frac{24\xi}{(1-\xi)^4 y^6} \Big(& (1+2\xi)^2 y^3 (\sin y - \cos y) \\ & - 6\xi \left(1 + \frac{\xi}{2}\right)^2 y^2 \left[2y\sin y - \left(y^2 - 2\right)\right] + \\ & \frac{\xi}{2}(1+2\xi)^2 \left[4y^3 - 24y\right]\sin y - \left(y^4 - 12y^2\right. \\ & \left. + 24\right)\cos y + 24]^{-1} \end{aligned} \tag{5}$$

And also, the structure factor equation with OCP method is mentioned below:

$$S(q) = \frac{S_0(q)}{1 + \rho\beta u^*(q) S_0(q)} \tag{6}$$

$$S_0(q) = \frac{1}{1 - \rho C_0(q)} \tag{7}$$

$$\begin{aligned} \rho C_0(q) = \frac{3\Gamma}{q^4 a^4 \alpha_2^2} & \left[\cos(qa\alpha_1) + 2\cos(qa\alpha_2)\right. \\ & \left. - \frac{3\sin(qa\alpha_1)}{qa\alpha_1}\right] \end{aligned} \tag{8}$$

where, α_1 and α_2 are the dimensionless parameters and also β $\mu^*(q)$ equations were taken from the mentioned reference [16–18] for the static structure factor of the OCP reference system. Here while deriving the static structure factor using OCP system, we have used our own developed model pseudopotential.

2.1 Phonon dispersion relation

Finding a single model potential that can be used to precisely compute a variety of material properties is challenging. Problems arise when the physical phase shifts from solid to liquid or the other way around. In other words, not all of the properties in the liquid state can be achieved by the potential provided for the solid. We propose a new potential as stated in Eq (3) to get around this problem and evaluate the phonon dispersion curves and other vibrational properties. To compute the phonon dispersion relations of liquid metals, the most frequently used approach of Hubbard and Beeby [6] is adopted for the calculations. With the physical argument that the product of the static pair correlation function $g(r)$ and the second derivative of the interatomic pair potential $\phi(r)$ is peaked near the hard sphere diameter . Hubbard and Beeby [6] have derived the equations for the longitudinal phonon frequencies $\omega_L(q)$ and transverse phonon frequencies $\omega_T(q)$ as:

$$\begin{aligned} {\omega_L}^2(q) = {\omega_E}^2 [1 - \frac{3\sin(q\sigma)}{q\sigma} - \frac{6\cos(q\sigma)}{(q\sigma)^2} \\ + \frac{6\sin(q\sigma)}{(q\sigma)^3}] \end{aligned} \tag{9}$$

and

$$\omega_T^2(q) = \omega_E^2 \left[1 + \frac{3\cos(q\sigma)}{(q\sigma)^2} - \frac{3\sin(q\sigma)}{(q\sigma)^3}\right] \tag{10}$$

In the above mentioned equations ω_E represents the maximum phonon frequency and is given as,

$$\omega_E = k \int_0^\infty g(r) r^2 \phi''(r) dr \tag{11}$$

with

$$k = \frac{4\pi\rho}{3M} \tag{12}$$

$$\begin{aligned} \phi''(r) = \frac{4Z^2}{r^3} + \frac{\Omega}{\pi^2} \int_0^\infty F(q) q^2 \left[\frac{2\sin(qr)}{qr^3} - \frac{2\cos(qr)}{qr^3}\right. \\ \left. - \frac{q\sin(qr)}{r}\right] dq \end{aligned} \tag{13}$$

with $\phi''(r) = \frac{\partial^2 \phi(r)}{\partial r^2}$
The energy wave number characteristics $F(q)$ in the above equation can be written as,

$$F(q) = -\frac{\Omega_0 q^2}{16\pi} |V(q)|^2 \frac{[\varepsilon_H(q) - 1]}{1 + [\varepsilon_H(q) - 1][1 - f(q)]} \tag{14}$$

In the above equation $V(q), \varepsilon_H(q), F(q)$ are the bare ion potential, modified Hartree dielectric function and local field correction functions, respectively.

The exchange and correlation screening functions from Hartree [21], Taylor [22], and Nagy [23] were utilized here to calculate the aforementioned properties. The Hartree screening function is purely static and it does not include any exchange and correlation effects. The expression for it as:

$$f(q) = 0 \tag{15}$$

The Taylor local field correction function [22] is a simple formula for static electron gas dielectric function, incorporating exchange and correlation effects, which generates calculated physical properties with good precession and justification. The equation for the function is follows:

$$f(q) = \frac{q^2}{4k_F^2}\left[1 + \frac{0.1534}{\pi k_F}\right] \tag{16}$$

Nagy local field correlation function [23] is used in the static mean field approximation the result is analytic and depends upon the value of the pair-correlation function at zero inter-particle separation. This analytic equation can be written as:

$$f(q) = 1 - g(0,n) + \frac{cb}{c^2+q^2} - \frac{g(0,n)}{q}\tan^{-1}\left(\frac{q}{c}\right) \tag{17}$$

The parameters $g(0,n)$and c were taken as mentioned in the original article [23].

2.2 Elastic constants and parameters

In addition to phonon dispersion curves, the current study has been expanded to determine a few constants and parameters required to provide a full bulk of liquid alkali metals. The usual equations are used to calculate the aforementioned parameters.

In the long-wavelength limit of the frequency spectrum, the both frequencies i.e. transverse and longitudinal are proportional to the wave vectors and obey the relations.

$\omega_L \propto q$ and $\omega_T \propto q$

$$\omega_L = v_L q \quad \mathit{and} \quad \omega_T = v_T q \tag{18}$$

where, v_L and v_T are the longitudinal and transverse sound velocities of the liquid metals respectively. Equations for v_L and v_T are given by,

$$v_L = \omega_E\sqrt{\frac{3\sigma^2}{10}} \quad \mathit{and} \quad v_T = \omega_E\sqrt{\frac{\sigma^2}{10}} \tag{19}$$

Various elastic properties are then determined by the longitudinal and transverse phonon frequencies. The bulk modulus (B), modulus of rigidity (G), Young's modulus (Y) [24] and Debye temperature θ_D [24] are calculated using following expressions,

$$B_T = \rho v_L^2 - \frac{4v_T^2}{3}, \quad G = \rho v_T^2, \quad Y = 2G(\sigma+1) \tag{20}$$

$$\sigma = \frac{1 - 2\left(\frac{v_T^2}{v_L^2}\right)}{2 - 2\left(\frac{v_T^2}{v_L^2}\right)} \tag{21}$$

The Debye temperature is given in terms of both the velocities as [24],beg

$$\theta_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar}{k_B}2\pi\left[\frac{9\rho}{4\pi}\right]^{1/3}\left[\frac{1}{v_L^3} + \frac{2}{v_T^3}\right]^{-1/3} \tag{22}$$

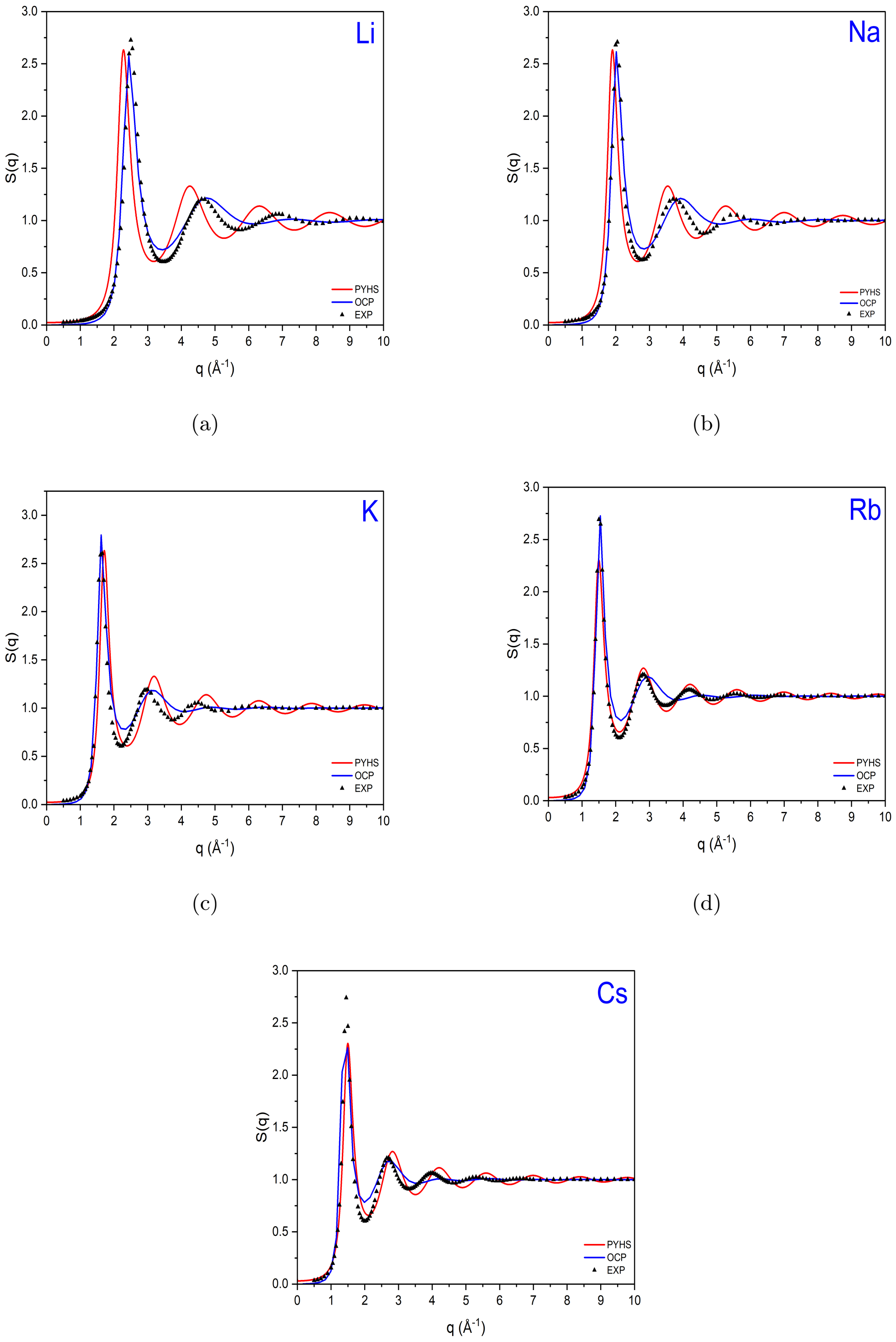
Here $\hbar$ represents the Planck constant, k_B the Boltzmann constant, ω_D the Debye frequency, and ρ the number density, respectively. Here, θ_D shows the characteristic atomic motions in the liquid phase and is assumed to be constant over the temperature range of interest. For liquid metals, it is often treated as a parameter and fixed with the help of equation (14).

3 Results and Discussion

The input parameters used in the present computation are tabulated in Table 1 which are directly taken from [25, 26]. The parameters of the model potential are considered from Eq. (4).

Table 1: Input parameters and constants

Metal	Z	Π_0 (au)	$T(K)$	ξ	r_c	Γ
Li	1	151.82	453.0	0.46	1.4649	210.75
Na	1	277.51	378.0	0.46	1.7925	206.45
K	1	529.63	343.0	0.46	2.1877	183.35
Rb	1	648.68	313.0	0.43	2.3901	187.86
Cs	1	810.06	303.0	0.43	2.5539	180.21



(a)

(b)

(c)

(d)

(e)

Figure 1: Structure factor comparison for PYHS and OCP methods for (a) Li, (b) Na, (c) K, (d) Rb, (e) Cs

Here, Z, Π_0, T, ξ, r_c and Γ are valence, atomic volume, temperature, packing fraction, pseudopotential parameter, and plasma component, respectively. The respective structure factors for the liquid metals Li, Na, K, Rb, and Cs are shown in Figure 1. Three distinct types of techniques, including PYHS and OCP, were employed to compute the structure factors using the newly proposed pseudopotential. The currently available experimental structure factor data [27] and the computed structure factor graphs have been compared in Figure 1. As shown in Figure 1 for the metals under study, the pseudopotential has proven to have extremely good agreement with the current experimental results [27]. As can be shown, both methodologies for every ingredient offer superb agreement with experimental findings [27]. It can therefore be inferred that the recently created pseudopotential is particularly useful in evaluating a number of liquid metal properties. All of the information we utilized in this post was obtained using the melting point temperature.

Tables 2 and 3 compare the locations of the first and second peaks as well as the corresponding magnitudes of structure factors.

According to Waseda [27], the hard sphere structure factor shows the following features:

1. The first peak of the structural factor is symmetrical.
2. A packing fraction $\xi = 0.45$ is determined to have the best agreement with experimental data at temperatures just above the melting point.
3. The ratio of the second peak's position to the first peak, α, is roughly 1.86.

Thus, the measured deviation from the hard-sphere structure factor gives useful information in the structural study of liquid metals. Therefore, from Fig. 1, it has been observed that both the structure factor models give very good qualitative data in comparison with the available experimental data [27]. From the results of the first and second peak positions of the structure factor narrated in Table 2, quite good agreement with the experimental value [27] due to OCP was found in comparison with PYHS. So, the ratio mentioned in Table 3 calculated by both the structure factor methods is found to be consistent with experimental outcomes given in the literature [27].

It has been established that both the structure factor data are qualitatively consistent with the experimental findings [27]. As a result, when compared to the PYHS reference system, the OCP reference system gives a more accurate representation of the structure of monovalent metals. According to our research, PYHS is less useful than the OCP reference system for comprehending the structural behavior of liquid metals. The results also support the study's usage of the newly created pseudopotential.

The pair correlation function is also an important component while examining the vibrational properties of liquid metals, as it provides the statistical description of the structure of liquid metals. The g(r) has also been determined using the earlier estimated values of the structure factor. The phonon dispersion curves were generated using the various structure factor approaches in accordance with Eq. (1) above, and they were contrasted with the available experimental data [27].

Table 2: Comparison for the first peak positions of structure factors

Metal	First Peak position and Related Magnitude in $S(q)$					
	Peak Position in (Å^{-1})			Related Magnitude		
	PYHS	OCP	EXPT.[27]	PYHS	OCP	EXPT.[27]
Li	2.29	2.44	2.50	2.62	2.57	2.72
Na	1.91	2.01	2.05	2.63	2.61	2.70
K	1.70	1.62	1.65	2.62	2.79	2.60
Rb	1.48	1.54	1.50	2.29	2.72	2.69
Cs	1.48	1.49	1.45	2.30	2.26	2.73

Table 3: Comparison for the second peak positions of structure factors

Metal	Second Peak position and Related Magnitude in S(q)					
	Peak Position in (Å^{-1})			Related Magnitude		
	PYHS	OCP	EXP. [27]	PYHS	OCP	EXP. [27]
Li	4.28	4.74	4.70	1.32	1.21	1.20
Na	3.59	3.91	3.80	1.32	1.21	1.19
K	3.21	3.09	3.00	1.31	1.18	1.19
Rb	2.85	2.92	2.80	1.26	1.19	1.20
Cs	2.86	2.81	2.70	1.25	1.17	1.20

Table 4: Ratio of the structure factor S(q)

Metal	PYHS	OCP	EXP. [27]
Li	1.86	1.94	1.88
Na	1.87	1.90	1.85
K	1.88	1.90	1.81
Rb	1.92	1.89	1.86
Cs	1.93	1.88	1.86

Table 5: Comparison of first peak positions and related magnitudes in $g(r)$ for different metals.

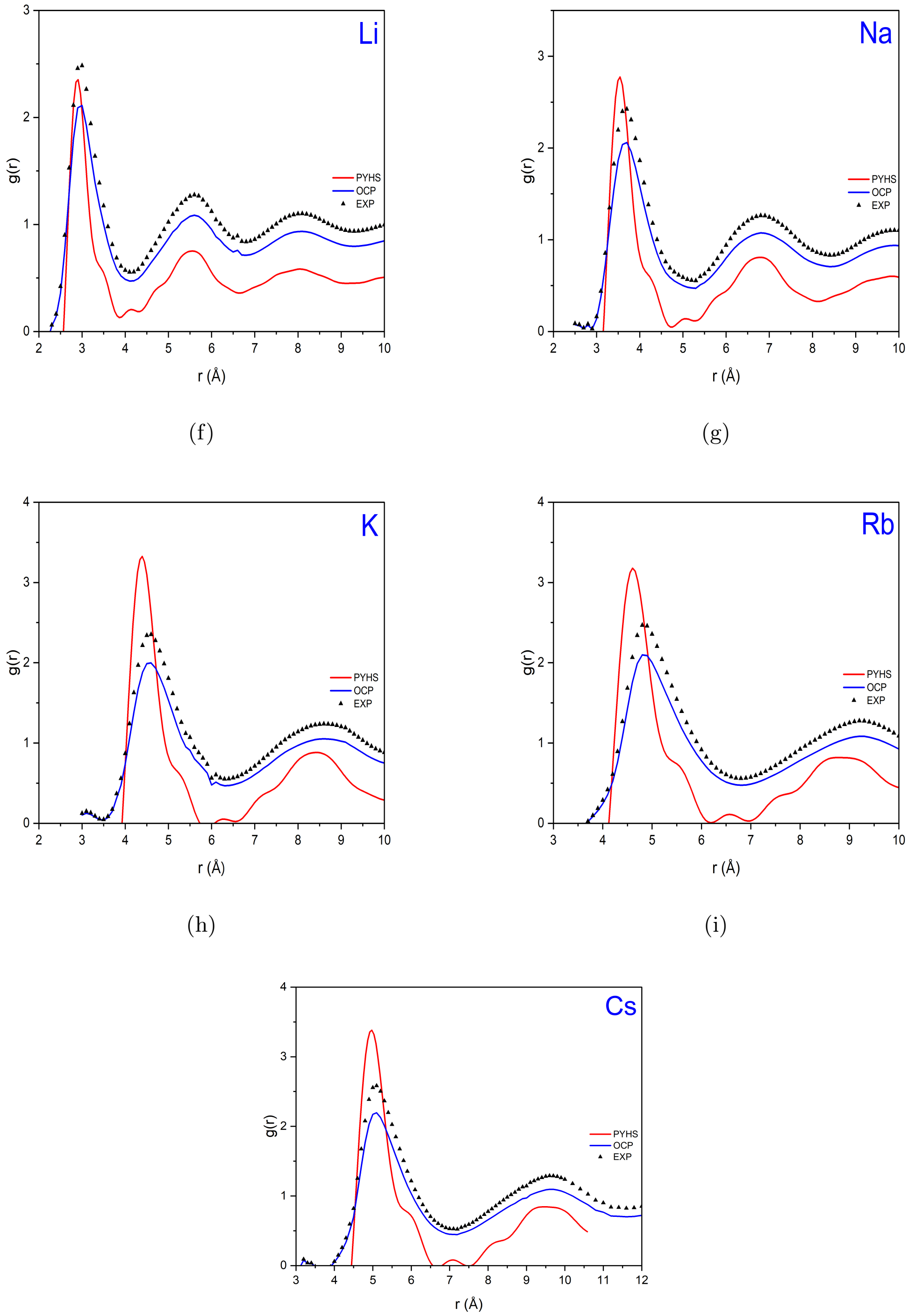
Metal	Second Peak position and Related magnitude in g(r)					
	Peak Position in (Å^{-1})			Related Magnitude		
	PYHS	OCP	EXP. [27]	PYHS	OCP	EXP. [27]
Li	2.91	3.00	3.00	2.35	2.11	2.48
Na	3.54	3.70	3.70	2.77	2.06	2.42
K	4.39	4.60	4.60	3.32	2.00	2.35
Rb	4.60	4.80	4.80	3.17	2.10	2.47
Cs	4.97	5.12	5.10	3.38	2.19	2.58

Table 6: The comparison for the second peak positions of $g(r)$.

Metal	First Peak position and Related magnitude in g(r)					
	Peak Position in (Å^{-1})			Related Magnitude		
	PYHS	OCP	EXP. [27]	PYHS	OCP	EXP. [27]
Li	5.60	5.72	5.70	0.74	1.07	1.22
Na	6.82	6.80	6.80	0.81	1.07	1.26
K	8.47	8.70	8.70	0.89	1.05	1.23
Rb	8.83	9.20	9.20	0.82	1.08	1.28
Cs	9.52	9.60	9.60	0.84	1.09	1.30

Table 7: The ratio (r_1/r_2) for the pair distribution function $g(r)$.

Metal	PYHS	OCP	EXP. [27]
Li	1.92	1.90	1.90
Na	1.92	1.83	1.83
K	1.92	1.81	1.81
Rb	1.91	1.91	1.91
Cs	1.92	1.88	1.88



(f) (g)

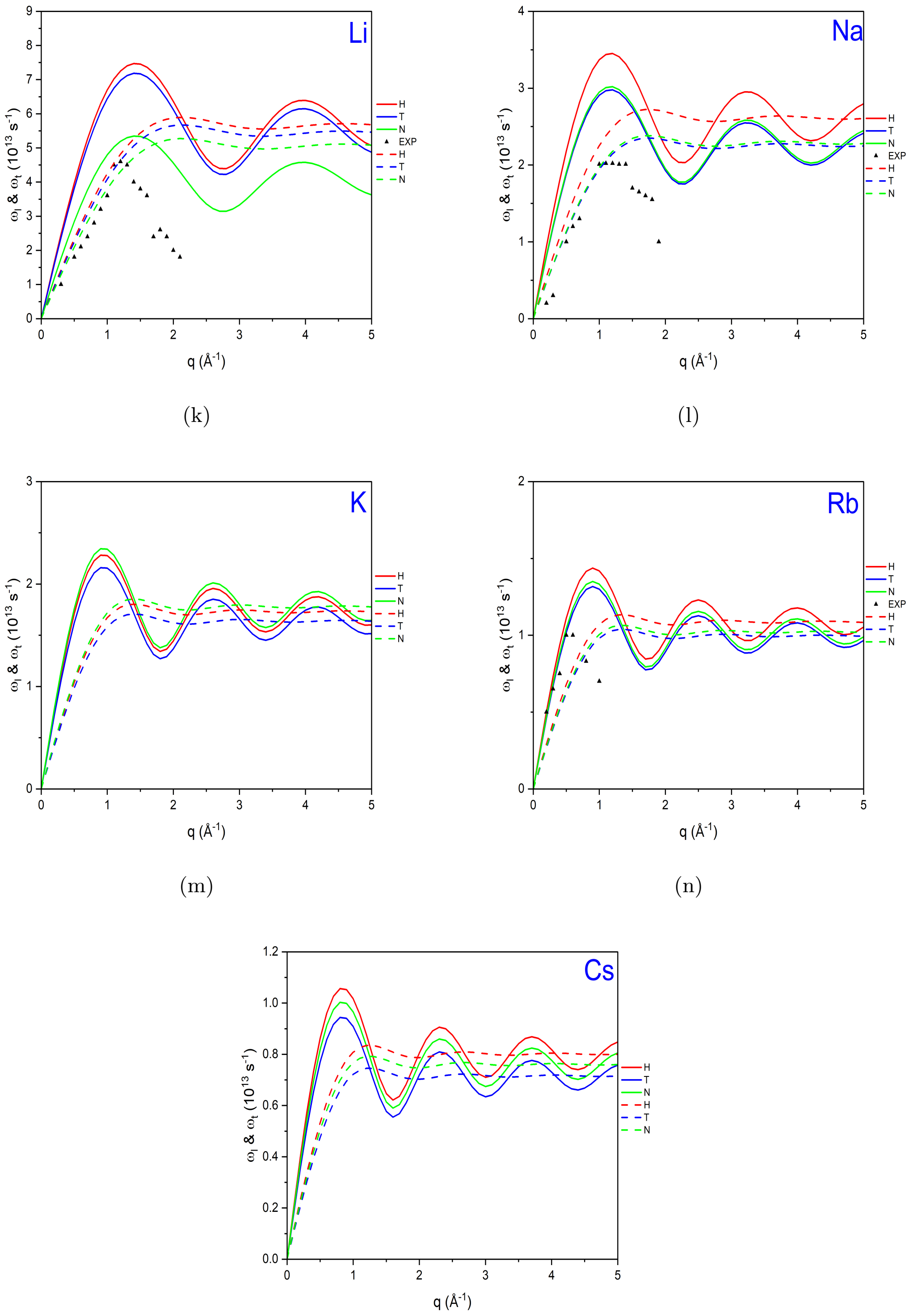
(h) (i)

(j)

Figure 2: Pair correlation function comparison for PYHS and OCP methods for (f) Li, (g) Na, (h) K, (i) Rb, (j) Cs.

In a system with average number density, the probability of finding another atom at a distance r from an origin atom corresponds to $g(r)$. The function $g(r)$ is called the pair correlation function and is frequently used for the discussion of non-crystalline systems. The information given by $g(r)$ is only single-dimensional, but it does provide quantitative information on non-crystalline systems [27]. Therefore, the pair correlation function is one of the most important pieces of information in this study.

When compared to the PYHS technique, the pair distribution functions from various reference



(k)

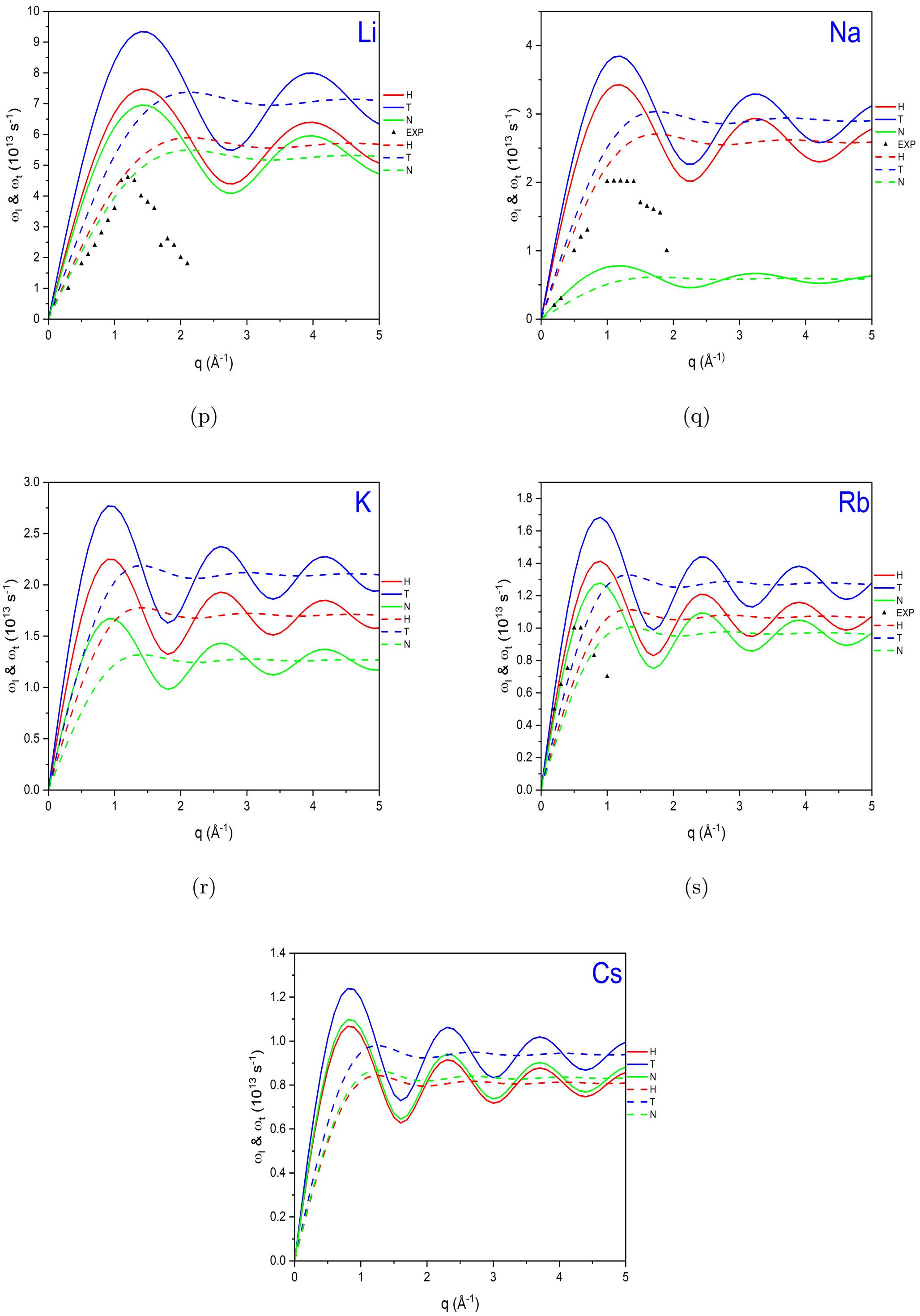
(l)

(m)

(n)

(o)

Figure 3: The phonon frequencies (solid line), (dashed line) of different element using PYHS structure factor for (k) Li, (l) Na, (m) K, (n) Rb and (o) Cs.

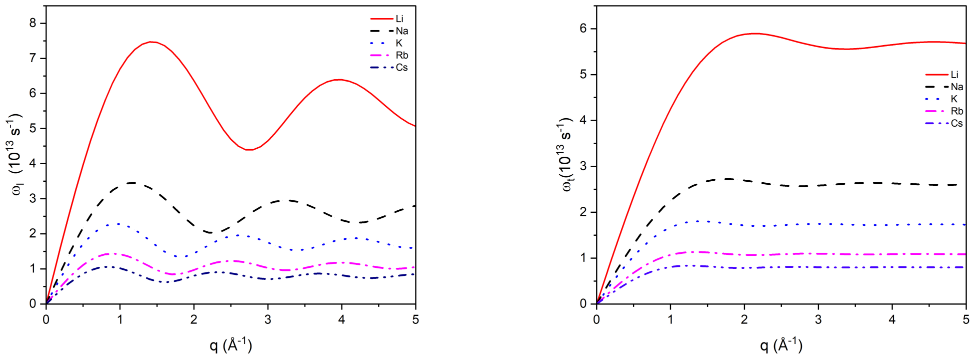


(p) (q)

(r) (s)

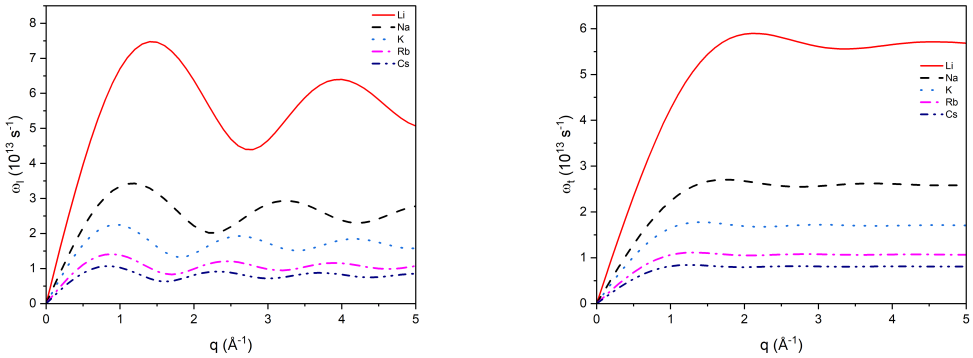
(t)

Figure 4: The phonon frequencies (solid line), (dashed line) different elements using OCP structure factor for (p) Li, (q) Na, (r) K, (s) Rb and (t) Cs



(a) (b)

Figure 5: Metal wise comparison for ω_l and ω_t with PYHS method.



(c) (d)

Figure 6: Metal wise comparison for ω_l and ω_t with OCP method.

systems show that the OCP method is considerably more in line with the experimental data [27].

The percentage variation in the first peak position q_1 of the structure factor using the PYHS model with the experimental data [27] for the given elements were found to be 1.33%–12.4%, whereas for the OCP method it was calculated as 1.33%–2.75%. For the second peak variation q_2, the PYHS model gives 0.77%–18.58%, while the OCP calculation gives a variation of 1.11%–17.21% and 0.40%–9.36%, respectively, with the experimental data [27].

For the first peak of the pair correlation function $g(r)$, the variation found for the PYHS and OCP methods for the liquid alkali metals were 2.35%–4.56% and 0.00%–0.39%, respectively. For the second peak variation $g(r)$, the above-mentioned models yield 0.29%–5.40% and 0.00%–0.35%, respectively.

For all liquid alkali metals, the longitudinal vibration variation with regard to the wave vector, calculated using the PYHS and OCP structure factors, was examined in 3 and 4. The findings of various local field correction functions are displayed using colour coding. For the PYHS method, one can see that the Hartree function [21] gives the highest value for $\omega_L(q)$ and $\omega_T(q)$ for all the elements except K because, for element K, the screening function of Nagy [23] gives the least values. Also, there are experimental data available for Li, Na, and Rb [28,29] elements, so the comparison is also shown in the same Figures 3 and 4. It shows that our obtained results are in qualitative agreement with the available experimental data [28,29]. Also, for the elements, $\omega_L(q)$ shows more oscillatory behaviour in comparison with $\omega_T(q)$. In the discussion for $S_T(q)$, less oscillatory behaviour was observed, and one can see that the screening function of Taylor [22] gives the maximum value for all the elements, while Nagy [23] gives the least value except for Cs. In Cs, the Hartree [21] screening function shows the least results, which are very similar to the data with Nagy [23].

Figure 6 shows that at larger q values, greater oscillatory behaviour is found in the case of $\omega_L(q)$ than in the case of $\omega_T(q)$ with different structure

Table 8: Vibrational properties of liquid metals with PYHS structure factor

Parameters	Results	Li	Na	K	Rb	Cs
$v_L \times 10^3$cm/s	H	8.3761	4.7317	3.8865	2.5546	2.0273
	T	8.0555	4.0830	3.6797	2.3418	1.8110
	N	5.9971	0.8279	2.2189	1.7778	1.6037
	Exp. [30]	-	2.51	-	-	-
	Others[12,13]	8.88, 8.61	3.77, 4.41	3.01, 2.97	1.92, 1.90	1.48, 1.44
$v_T \times 10^3$cm/s	H	4.8359	2.7318	2.2439	1.4749	1.1704
	T	4.6508	2.3573	2.1245	1.3520	1.0455
	N	3.4624	0.4780	1.2810	1.0264	0.9259
	Exp. [30]	-	1.81	-	-	-
	Others[12,13]	5.13, 4.97	2.18, 2.54	1.74, 1.69	1.11, 1.08	0.85, 0.83
G dyne/cm^2	H	1.2079	0.6928	0.4153	0.3210	0.2518
	T	1.1172	0.5159	0.3723	0.2698	0.2009
	N	0.6192	0.0212	0.1353	0.1554	0.1575
	Others[12,31]	14.10, 13.25	4.41, 6.54	2.76, 2.59	2.01, 1.90	1.45, 1.39
B$\times 10^3$dyne/cm^2	H	2.013	1.1547	0.6922	0.5351	0.4196
	T	1.8620	0.8598	0.6205	0.4496	0.3348
	T	1.0324	0.0353	0.2256	0.2591	0.2626
	Exp. [12]	-	5.3	-	-	-
	Others [12, 31]	2.35, 2.21	7.35, 1.09	0.46, 0.43	0.33, 0.32	0.24, 0.23
Y$\times 10^{11}$dyne/cm^2	H	3.0197	1.7321	1.0383	0.8026	0.6294
	T	2.7930	1.2897	0.9307	0.6745	0.5023
	N	1.5480	0.0530	0.3384	0.3887	0.3939
	Others [12, 31]	3.53, 3.18	1.10, 1.64	0.69, 0.65	0.50, 0.47	0.36, 0.35
θ_D(K)	H	566.4771	261.7193	173.3101	106.4724	78.4634
	T	544.7990	225.8393	164.0891	97.6051	70.0914
	N	405.5852	45.7920	98.9458	74.0991	62.0717
	Others [12, 32, 33]	609.80, 579.46	250.85, 240.35	138.77, 134.45	82.82, 80.56	58.81, 58.46

factor methods of PYHS and OCP. This assures that longitudinal phonons alone, and not both, are responsible for group oscillations. The linear response exists in phonon dispersion curves at low q values but vanishes at larger q. This happens as a result of the velocity altering as q shifts. Because all of the metals under examination, due to the Hartree [21] screening function, exhibit identical oscillating behaviour, the Hartree-Bogolyubov (HB) approach yields reasonably fruitful results. Additionally, Li exhibits the maximum vibrations for all the different structure factor techniques for liquid alkali metals, but Cs gives the lowest vibrations.

The vibrational properties of all the above-mentioned liquid metals are shown in Tables 8-10. The parameters include the longitudinal velocity of sound (v_L), transverse velocity of sound (v_T), modulus of rigidity (G), isothermal bulk modulus (B), Young's modulus (Y), and Debye temperature (θ_D). The selected liquid alkali metals show screening sensitivity in the low-momentum region. Furthermore, the phonons can be detected as sound waves thanks to the spectrum's macroscopic frequency limit. As a result, the longitudinal and transverse sound velocities have been calculated using the linear component of their dispersion curves. Both structure factor techniques' predictions for vibrational properties are found to be qualitatively consistent with the theoretical or experimental findings detailed in the literature [12]. To put it another way, a property essentially has the same value for all permutations of the structure factor method, but divergence is apparent when using the screening functions. One can observe that for both methods exceptionally well results in agreement with the experimental values for v_L and v_T. Hence, PYHS and OCP structure factor techniques for calculating the isothermal bulk modulus B provide findings that are qualitatively consistent with the experimental data for all Na. Similar results were found for Li, K, Rb, and Cs as individual elements using both structure factor approaches as well as experimental data [30–35].

Table 9: Vibrational properties of liquid metals with OCP structure factor

Parameters	Results	Li	Na	K	Rb	Cs
$v_L \times 10^3$cm/s	H	8.3797	4.6998	3.8307	2.5699	2.0480
	T	8.0590	4.0555	3.6269	2.3559	1.8295
	N	5.9996	0.8223	2.1870	1.7885	1.6202
	Exp. [30]	-	2.51	-	-	-
	Others [12, 31]	8.88, 8.61	3.77, 4.41	3.01, 2.97	1.92, 1.90	1.48, 1.44
$v_T \times 10^3$cm/s	H	4.8320	2.7134	2.2117	1.4870	1.1824
	T	4.6528	2.3414	2.0940	1.3601	1.0562
	N	3.4639	0.4747	1.2626	1.0326	0.9354
	Exp. [30]	-	1.81	-	-	-
	Others [12, 31]	5.13, 4.97	2.18, 2.54	1.74, 1.69	1.11, 1.08	0.85, 0.83
G dyne/cm^2	H	1.1987	0.6832	0.4043	0.3249	0.2569
	T	1.1087	0.5087	0.3624	0.2730	0.2050
	N	0.6145	0.0209	0.1318	0.1573	0.1608
	Exp. [12]	-	5.3	-	-	-
	Others [12, 31]	14.10, 13.25	4.41, 6.54	2.76, 2.59	2.01, 1.90	1.45, 1.39
B$\times 10^3$dyne/cm^2	H	1.9979	1.1387	0.6739	0.5413	0.4282
	T	1.8479	0.8479	0.6041	0.4551	0.3418
	N	1.0241	0.0348	0.2196	0.2623	0.2680
	Exp. [12]	-	5.3	-	-	-
	Others [12, 31]	2.35, 2.21	7.35, 1.09	0.46, 0.43	0.33, 0.32	0.24, 0.23
Y$\times 10^{11}$dyne/cm^2	H	2.9968	1.7081	1.0109	0.8123	0.6424
	T	2.7719	1.2719	0.9061	0.6826	0.5126
	N	1.5362	0.0523	0.3295	0.3934	0.4020
	Others [12, 31]	3.53, 3.18	1.10, 1.64	0.69, 0.65	0.50, 0.47	0.36, 0.35
θ_D(K)	H	566.7200	259.9579	170.8222	107.1108	79.2655
	T	545.0326	224.3194	161.7336	98.1903	70.8080
	N	405.7591	45.4868	97.5255	74.5434	62.7063
	Others [12, 32, 33]	609.80, 579.46	250.85, 240.35	138.77, 134.45	82.82, 80.56	58.81, 58.46

The additional theoretical data [12, 32–35] for the modulus of rigidity G for all the elements available in the literature for comparison, and both structure factor approaches were determined to be appropriate to derive the same property. Similar to Young's modulus, the statistics for all the elements were accessible, which were determined to be good in comparison to the same, and the most recent estimated Debye temperature θ_D is extremely similar to the values actually obtained. With all three types of screening functions, it is discovered that the data obtained by the three structure factor methods are quite similar to one another.

4 Conclusion

From the above comprehensive study, it can be concluded that the structural and vibrational properties, i.e., phonon dispersion curves (PDC), longitudinal sound velocity (v_L), transverse sound velocity (v_T), isothermal bulk modulus (B), modulus of rigidity (G), Young's modulus (Y), Debye temperature (θ_D) of some monovalent (Li, Na, K, Rb, Cs) liquid metals using the newly developed model potential with the two different types of structure factor methods PYHS and OCP, with three types of screening functions, namely Hartree (H), Taylor (T), and Nagy (N), are reported for the first time. It can be challenging to decide which structure factor methodology is most appropriate for computing the vibrational properties of liquid metals because each of the three approaches employed here has its own distinct identity, significance, and limitations. However, from the obtained data, we can say that the HB approach calculates precise conclusions for phonon data with the fewest parameters possible, and the OCP method gives better results in comparison with the PYHS method. We conclude that the vibrational properties of the aforementioned liquid metals may be efficiently studied by PDCs derived from the HB technique with three local field correction functions, namely H, T, and N. These formulas accurately reproduce all of the salient features of phonon dispersion curves. Hence, the presently adopted model potential is found suitable when used in conjunction with the HB approach. The model potential provides less complex calculation of the vibrational properties of the metals under study as it is using only a single parameter (r_c). The obtained vibrational properties serve as a detailed database for further research in the field of liquid metals study.

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