Phonon modes in non-crystalline Lithium, Sodium and their binary alloys

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The longitudinal and transverse phonon modes of light weight non-crystalline alkali metals lithium, sodium and their binary alloy systems (viz. $Li_{0.50}Na_{0.50}$ and $Li_{0.69}Na_{0.31}$) are studied in terms of the eigen-frequencies of the localized collective excitations using pseudopotential formalism. The self-consistent phonon scheme involving multiple scattering and phonon eigen-frequencies, which are expressed in terms of many-body correlation functions of atoms as well as of inter-atomic potential, have been used. The pair potential is obtained by Wills Harrison (WH) form using model pseudopotential. Local field correlation functions due to Hartree (H), Taylor (T), Ichimaru and Utsumi (IU), Sarkar et al. (S) and Farid et al (F) are used to investigate influence of the screening effects on the vibrational properties. Results for phonon dispersion curves (PDC) are reported which are consistence with available experimental and other theoretical results confirming the applicability of model potential for such studies.

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1. Introduction

The non-crystalline substances are the basis for variety of bulk metallic glass forming systems, and efforts to optimize the properties of these materials have led to increasing interest in understanding the thermodynamic and kinetic properties of the liquid phases from which they are formed. The liquid phase is of particular interest since properties in this phase are relatively well characterized experimentally yet uncertainties persist in theoretical models of bonding, structure, and thermodynamical properties [1-2].

In recent years, neutron scattering data from short wavelength phonons in amorphous solids and liquids have become increasingly available. Quite significantly, the scattered neutron spectra of amorphous or crystalline solids near their melting point and that of liquids shows remarkable similarity [3]. The collective modes in liquids involve a cooperative motion of a system governed by the interaction between the particles and it seems that the system moves in its own self-consistent field. The existence of propagating collective modes of finite wavelength in liquid metals and their binary alloys are subject of growing interest [4]. The wavelengths of these modes are smaller than the interatomic spacing of the constituent combination of the liquid alloys. The measurements on liquid Pb near the freezing point were interpreted as evidence for the existence of both longitudinal and transverse modes, with wavelengths comparable to two interatomic spacing [5]. Other experiments have also supported the existence of such modes [6-10]. Theoretical calculations have also exhibited the existence of longitudinal and transverse phonon modes in liquid metals and their metallic complexes [11-14].

The collective modes in liquids have been studied experimentally, theoretically and by computer simulations since last two decades [6-16]. Number of efforts has been made to understand the dynamical properties of liquid metals both theoretically and experimentally. Among this the collective excitations in liquid alkali binary systems was studied by the pioneer work of Jacucci and McDonald [17] on binary Sodium–Potassium liquid alloys. After that, several other experimental [18] and theoretical studies [19-20], including molecular dynamics (MD) simulations [21-22] have been performed on non-crystalline alkali metals and their alloys. Besides the non-crystalline lithium and sodium, the binary combination of lithium-sodium alloys $Li_{0.5}Na_{0.5}$ and $Li_{0.61}Na_{0.39}$ are particularly interesting as foremost is equiatomic alloys and $Li_{0.61}Na_{0.39}$ is important due to its specific characteristic nature, known as ‘zero alloys’.

In recent times *ab-initio* molecular-dynamics simulation for liquid $Li_{0.61}Na_{0.39}$ binary alloys at various temperatures above and below the phase-separating temperature have been investigated by Senda et al [22]. It has been revealed from their study that near the phase-separating temperature, in the electron density distribution, the Li ions tend to assemble together in the region where the electron density is high. The relation between the ionic configuration and the electron density distribution thus obtained for the bulk liquid Li–Na alloys is similar to that obtained for the Li–Na cluster and hence divulges that this composition has the peculiar advantage that, due to the negative scattering length of Lithium, coherent scattering is only from concentration fluctuations, and the coefficient for scattering from number density fluctuations is zero and hence called ‘zero alloys’.

Few experimental studies like small angle x-ray scattering [23] and neutron diffraction studies [24] have examined the structure factor of this alloy. Recently, dynamical properties of liquid Li-Na alloy at `zero alloy' composition by orbital-free *ab-initio* molecular dynamics (OF-AIMD) [25] and memory function formalism [26] have also revealed the existence of propagating sound modes in the same. Most recently Pratap et al [27] have computed the phonon spectra for liquid Li, Na and $Li_{0.61}Na_{0.39}$ using model of Bhatia and Singh [28] and the obtained results were compared with the available data due to inelastic neutron scattering (INS) and inelastic x-ray scattering (IXS) experiments. The pseudopotential formalisms were employed with the structure factor generated through Ashcroft-Langreth [29] model. It is also confirmed from other such studies on non-crystalline substances that structure is an important aspect for the collective excitation in non-crystalline binary alloy [30].

The theory of lattice dynamics, which was thought to be applicable only in the cases of ordered solids, has found successful application in amorphous solids and liquids also. The approaches by Hubbard and Beeby (HB) [31], Takeno and Goda (TG) [32] and Bhatia and Singh (BS) [28] have gone a long way in describing the theory of collective motion in simple liquids. These independent model approaches have also proved to be effective for the computation of longitudinal and transverse phonon frequencies in the binary non-crystalline solids [14, 27, 30, 33]. Stimulated by these studies we report here the comprehensive study of the phonon modes and elastic constants of liquid lithium, sodium and their specific binary (i.e. $Li_{0.50}Na_{0.50}$ and $Li_{0.69}Na_{0.31}$) alloys by considering it as a one component fluid. The purpose of present study is to describe the effect of sodium concentration on the collective modes of binary Li-Na system as well as to study the relative effect of different local field correction functions on the aforesaid properties. This paper is prepared as follows. Section 2 deals with the form of the pair potential, model potential, structural aspect and phonon calculation approach for the non-crystalline binary alloy together with the parameterizations employed in calculation. Section 3 deals with the results and discussion. The overall conclusions are described in section 4.

2. Computational details

As mentioned earlier, there are basically three main theoretical approaches used to compute the phonon frequency of non-crystalline metals and alloys using model potentials; one is the phenomenological theory of HB [31] in the random phase approximation, according to which, liquid differs from a crystalline solid in two principal ways. Firstly, the atoms in the liquid do not form a regular array, i.e. they are disordered and secondly the atoms in the liquid move more freely than in the solid. The second approach is the quasi-crystalline approximation technique with interatomic pair potential developed by TG [32], in which the correlation function for the displacement of atoms itself depends on the phonon frequencies. And the third is by evaluation of force constants as was done by BS [28], which is based on following two assumptions: (1) The ions interact with a central pair wise potential, which is effective between the nearest neighbors only and (2) the force on an ion due to volume-dependent energies in the metal (kinetic and exchange energies of the conduction electrons, the ground-state energy of the electron, etc.) could be calculated using the Thomas-Fermi method. Recently, the BS model is also revised by Shukla and Campanha [34].

The HB theoretical model has been utilized here to generate the phonon dispersion curves (PDC) of light weight non-crystalline alkali metals and their alloys of specific concentration in the present computation.

2.1Pair potential

The effective ion-ion interaction is given as

$$V(r) = \frac{Z^2 e^2}{r} + \frac{2}{\pi}\int dq\, F(q) \exp(-iq.r) \tag{1}$$

In which $F(q)$ is energy wave number characteristics. The first term in above expression gives the Coulomb interaction between ions and the second term is due to the indirect interaction through the conduction electrons. This indirect interaction can be calculated using the energy wave number characteristics $F(q)$. The effective pair potential for the binary system can be obtained from the pair potentials of the single components which is given by the expression,

$$V(r) = C_A^2 V_{AA}(r) + 2C_A C_B V_{AB}(r) + C_B^2 V_{BB}(r) \tag{2}$$

Where, V_{AA} is the pair potential for the A-A component, V_{BB} for the B-B component and V_{AB} is for the A-B component in the binary system. C_A and C_B are the concentration of A and B type of component respectively, they are given by

$$C_A = \frac{(1-x)\Omega_A}{(1-x)\Omega_A + x\Omega_B} \tag{3}$$

$$C_B = \frac{x\Omega_B}{(1-x)\Omega_A + x\Omega_B} \tag{4}$$

Here Ω_A and Ω_B are the molar volume of the A and B components respectively. Another way of finding the pair potential for the binary alloy is to consider the system as a one component fluid. In the present study we have considered this effective atoms approach to compute the dispersion curves.

2.2 Model pseudopotential

The choice of model potential is an important aspect as it will describe the motion of valance electron in a metal. For the present study we have used single parametric local model pseudopotential of the following form in the r-space;

$$
\begin{aligned}
W_B(r) &= 0 && ; \quad for \quad r < r_c \\
&= -\frac{Ze^2}{r}\left[1-\exp\left(-{}^{r}\!/_{r_c}\right)\right] && ; \quad for \quad r \geq r_c
\end{aligned}
\qquad (5)
$$

This well tested model potential [35] is the modified version of Ashcroft's empty core model potential [36]. The potential is continuous in r- space and in comparison with Ashcroft empty core model potential, we have introduced $\frac{Ze^2}{r}\exp\left(-\frac{r}{r_c}\right)$ as a repulsive part outside the core which vanishes faster than only Coulomb potential $-\frac{Ze^2}{r}$ as $r \rightarrow \infty$. Moreover it may be noted that the inclusion of this repulsive term outside the core makes the effective core smaller than the ionic radius of the free electron. In the reciprocal space, the corresponding bare-ion form factor of the present model potential is given by:

$$
W_B(q) = \left(\frac{-4\pi Z e^2}{\Omega q^2}\right)\left[\cos\left(q r_c\right) - \left\{\frac{\left(q r_c\right)\exp\left(-1\right)}{1+q^2 r_c{}^2}\right\}\left\{\sin\left(q r_c\right) + \left(q r_c\right)\cos\left(q r_c\right)\right\}\right]. \qquad (6)
$$

Here, Z, e, Ω □ q and r_c are the valence, electronic charge, atomic volume, wave vector and the parameter of the potential, respectively. The energy wave number characteristics in expression (1) is given by,

$$
F(q) = -\frac{\Omega q^2}{16\pi}\left|W_B(q)\right|^2 \frac{\left[\varepsilon_H^{eff}(q)-1\right]}{\left[1+\left(\varepsilon_H^{eff}(q)-1\right)\left(1-f_{eff}(q)\right)\right]} \qquad (7)
$$

Here, $W_B(q)$ is the effective bare ion potential given by equation (6), $\varepsilon_H^{eff}(q)$ the Hartree dielectric response function and $f_{eff}(q)$ is the local field correction function used to introduce the exchange and correlation effects. The local field correction functions due to Hartree (H) [38], Taylor (T) [39], Ichimaru and Utsumi (IU) [40], Sarkar et al (S) [41] and Farid et al (F) [42] are used in the present study. The H function does not involve any exchange-correlation effect. Other four functions satisfy compressibility sum rule in the long wavelength limit. Table 1 contains the parameters used in the present computations.

Table 1. Input parameters used in the present calculations.

Element	Z	K_F (au)	r_c (au)	Ω_0 (au)^3	$r_{s\,(au)}$
Li	1	0.5890	1.00976	144.9	3.258
Na	1	0.4882	1.40459	254.5	3.931

2.3 Structure and pair correlation function

Pair potential or effective interaction is realized through interatomic potential (solid phase), ion-ion potential (liquid phase), and electron-electron potential developed between two similar particles like atoms, ions and electrons. In the study of non crystalline systems, the pair correlation function $g(r)$ is equally important as the pair potential. It contains useful information about the inter-particle radial correlation and structure which in turn decides the electrical, thermodynamical and other physical properties for crystals, liquid and amorphous materials. Experimentally, the function $g(r)$ can be obtained using X-ray diffraction and neutron scattering experiments and theoretically it is computed from different models, from effective pair potential and from *ab-initio* molecular dynamics.

One of the important properties while characterizing non-crystalline alloy is its static structure factor $S(q)$. It is a measure of particle correlation in the reciprocal space i.e. Fourier transform of $g(r)$. Most of the earlier attempts to compute structure factor $S(q)$ of liquid metals has the system of neutral hard sphere as their reference system. These models are quite useful for studying inert gas liquids, mono and poly-valent metals but do not give satisfactory results for some transition and rare earth metals. Among these the Ashcroft and Lekner (AL) model [29] is very effortless and more generally used model in early period of time. Since the non-crystalline binary alloy of Li-Na exhibits typical phase separation tendency we thought it worthwhile to compute structure factor $S(q)$ using AL model.

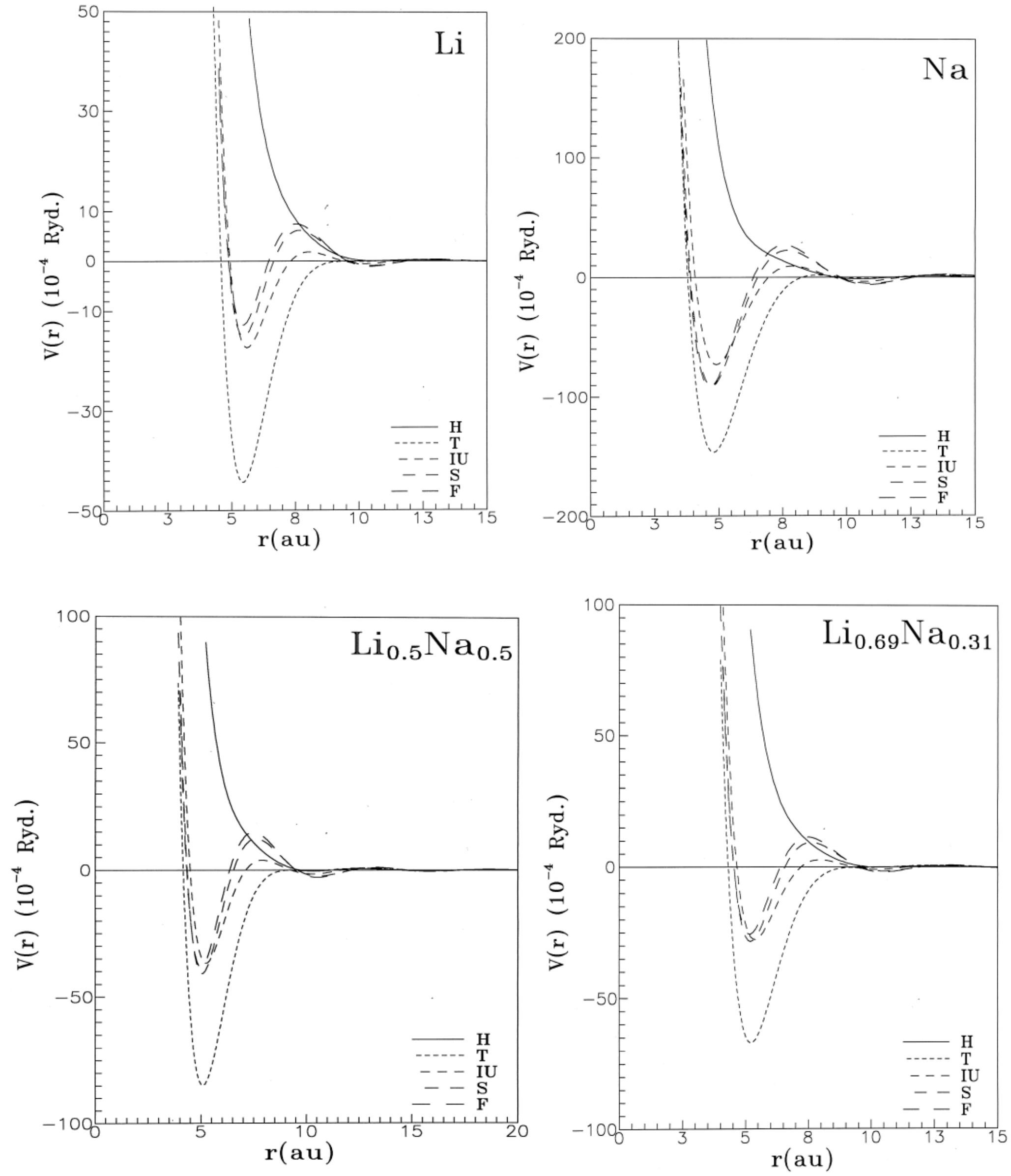

Fig. 1(a) Pair Potential for Li., (b) Pair potential for Na, 1(c) Pair potential for Li$_{0.5}$Na$_{0.5}$. 1(d) Pair potential for Li$_{0.61}$Na$_{0.39}$

Earlier, the partial structure factors of a liquid Li-Na alloy were calculated by Hoshino et al [43] using pair potentials based on pseudopotentials and the hyper-netted chain approximation of classical liquid theory. The concentration fluctuations in the long-wavelength limit, in liquid Li-Na alloy using the Bhatia-March [44] was studied by Lad et al [45] using the first principle calculations. The effects of the choice of the input parameter, namely core radius, in the Ashcroft pseudopotential and different local field corrections to the dielectric function are the basis of their study.

They established that the Ashcroft potential with a suitable choice of the core radius (fitting procedure) is effective and the asymmetrical behaviour indicates the phase separation tendency in the Li-Na alloy. In the same line we have calculated partial structure factor using Faber-Ziman [46] model and the results are shown in Fig. 2 (a) and (b). Here pair correlation function for both the binary combinations are shown Fig. 2 (c).

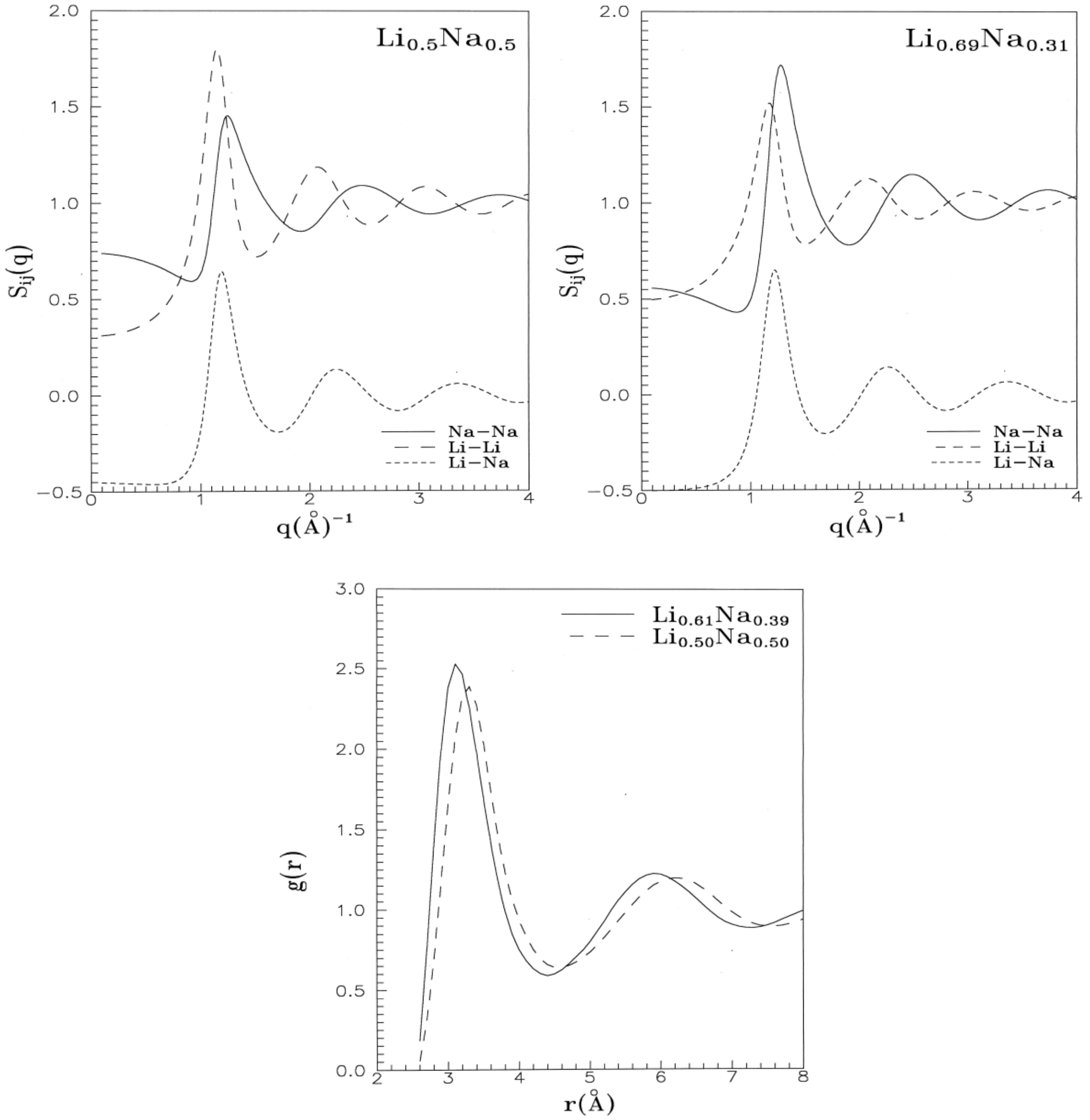

Fig. 2(a) Partial structure factor of Li.$_{05}$Na$_{0.5}$ binary alloy, (b) Partial structure factor of Li$_{0.61}$Na$_{0.39}$ binary alloy, (c) Pair correlation function for Li$_{0.5}$Na$_{0.5}$ and Li$_{0.61}$Na$_{0.39}$ alloys.

2.4 Phonon dispersion curves

The effective potential and pair correlation function $g(r)$ are then used to compute the longitudinal and transverse phonon frequencies. The product of the static pair correlation function '$g(r)$' and the second order derivative of the interatomic potential $V(r)$ is peaked at 'σ' which is the hard sphere diameter. The longitudinal phonon frequency $\omega_L(q)$ and transverse phonon frequency $\omega_T(q)$ are given by the expressions due to Hubbard and Beeby [31] as,

$$\omega_L^2(q)=\omega_E^2\left[1-\frac{3\sin(q\sigma)}{q\sigma}-\frac{6\cos(q\sigma)}{(q\sigma)^2}+\frac{6\sin(q\sigma)}{(q\sigma)^3}\right] \tag{8}$$

and

$$\omega_T^2(q)=\omega_E^2\left[1-\frac{3\cos(q\sigma)}{(q\sigma)^2}+\frac{3\sin(q\sigma)}{(q\sigma)^3}\right] \tag{9}$$

Where

$$\omega_E^2(q)=\frac{4\pi}{3M_{eff}\Omega}\int_0^\infty drg(r)r^2\frac{d^2V(r)}{dr^2} \tag{10}$$

is the maximum phonon frequency. The upper limit of the integration is decided by the length of the $g(r)$ used in the computation. M_{eff} is the effective atomic mass given by,

$$M_{eff}=(1-x)M_A+xM_B \tag{11}$$

Here M_A and M_B represents the atomic masses of the pure A and B components of the alloy respectively.

3. Results and discussion

In the present study, modified version of Ashcroft's potential is used to generate pair potential for the non-crystalline Lithium, Sodium and their binary alloy. The calculated pair potentials for liquid lithium, sodium and the combination of the binary alloys viz. $Li_{0.50}Na_{0.50}$ and $Li_{0.69}Na_{0.31}$ are shown in figures 1(a), 1(b), 1(c) and 1(d) using the aforesaid screening functions, respectively. A study shows that the general trend of the pair potentials in all the cases is same but the position of the first minima is greatly affected by the type of screening used.

The pair correlation function $g(r)$ is calculated from the structure factor $S(q)$. It is confirmed here that FZ model is successful in evaluating the partial structure factor and hence total structure factor. The computed partial structure factors for both alloys and pair correlation functions are shown in figures 2(a), 2(b) and 2(c), respectively.

The pair correlation function $g(r)$ has been derived from the structure factor and using the same, we have estimated the longitudinal and transverse phonon frequencies for binary alloys. The longitudinal and transverse phonon frequencies for Li, $Li_{0.50}Na_{0.50}$, $Li_{0.69}Na_{0.31}$ and Na are shown in Figures 3(a), 3(b), 3(c), 3(d) and Figures 4(a), 4(b), 4(c), 4(d), respectively.

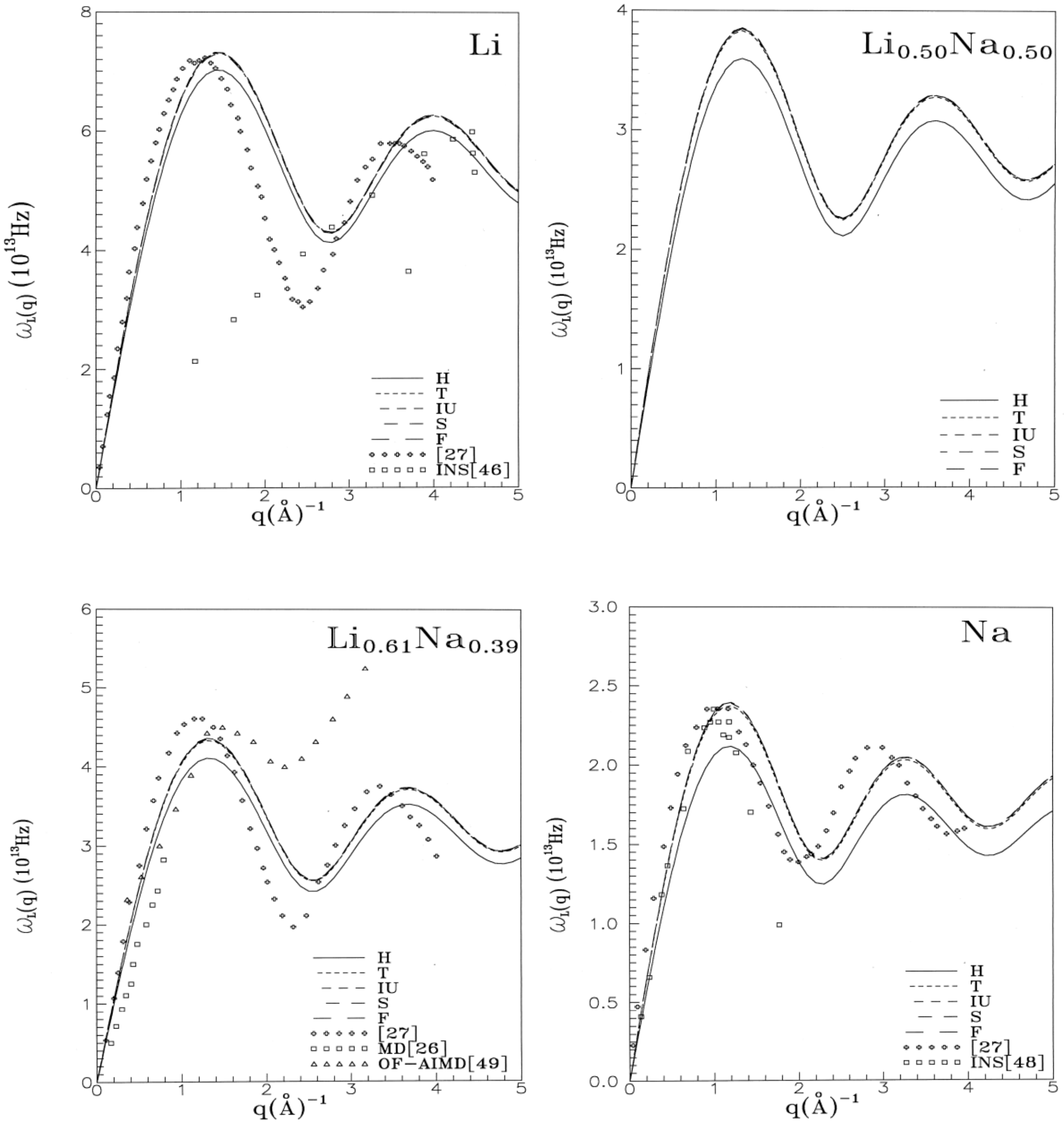

Fig. 3(a) Longitudinal phonon frequencies for Li, (b) Longitudinal phonon frequencies for $Li_{0.5}Na_{0.5}$, (c) Longitudinal phonon frequencies for $Li_{0.61}Na_{0.39}$, (d) Longitudinal phonon frequencies for Na

It is evident from the figures that the nature of peak positions are not much affected by different screening functions but both the transverse and longitudinal frequencies show deviation by using T, IU, SS and F with respect to H screening functions. It is obvious from the figures that the oscillations are prominent in the longitudinal mode as compared to transverse mode which indicates that the collective excitations at larger wave vector transfers due to the dispersion of longitudinal excitation. On the other hand the transverse modes undergo larger thermal modulation due to the anharmonicity of the vibrations in the alloy.

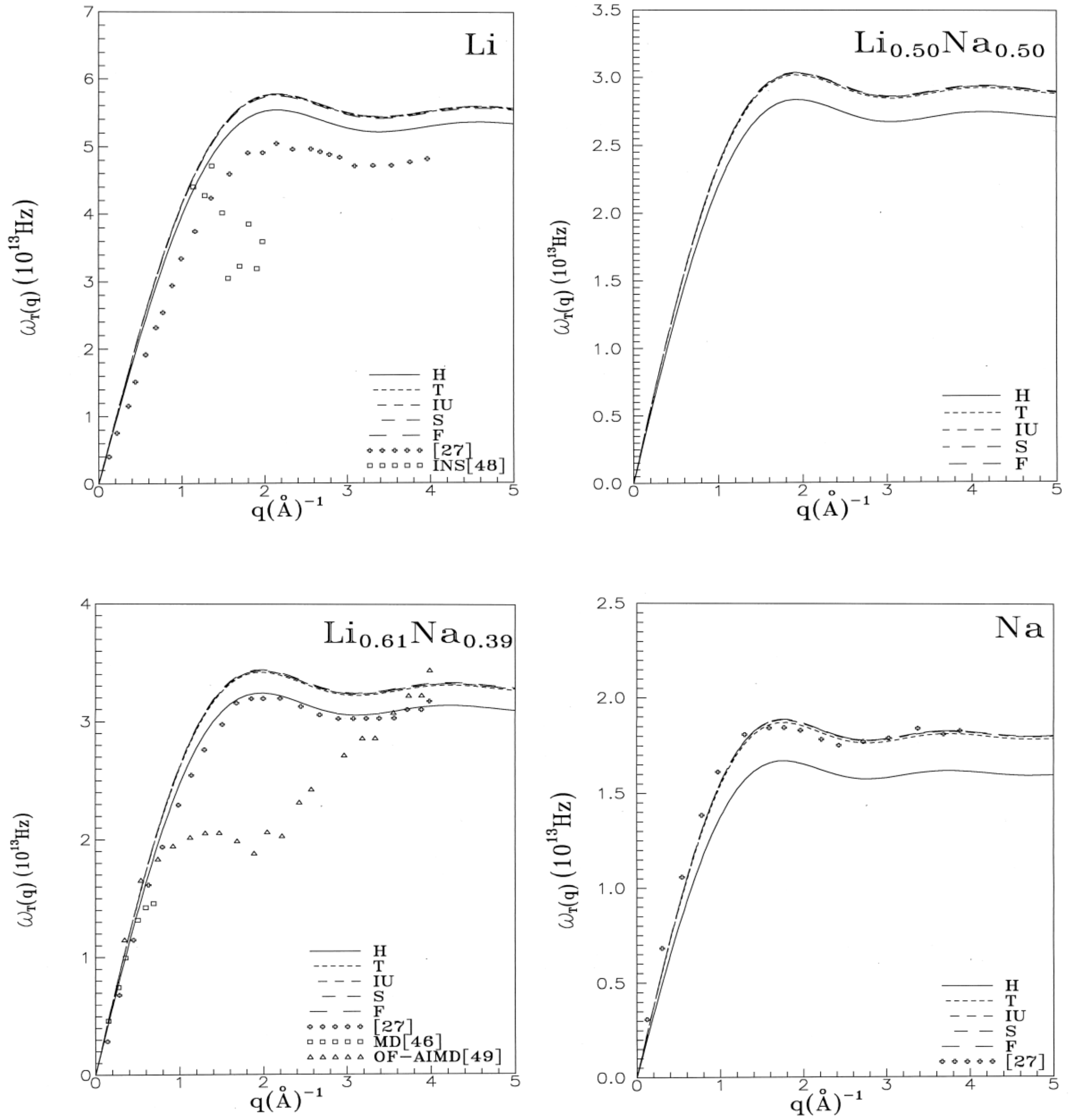

Fig. 4(a) Transverse phonon frequencies for Li, (b) Transverse phonon frequencies for Li$_{0.5}$Na$_{0.5}$ alloy, (c) Transverse phonon frequencies in Li$_{0.61}$Na$_{0.39}$ alloy, (d) Transverse phonon frequencies in Na

It can also be seen that the first minimum in the longitudinal branch of the dispersion curve falls at a value 2.5Å^{-1}, near which the static structure factor shows its principal peak. In the long wavelength limit the dispersion curves are linear and confirming characteristics of elastic waves.

The PDC for transverse modes attain maxima at a highrer q value than the longitudinal modes. As the concentration of Li increases, the phonon modes get supressed. This is because of the increase of atomic mass of the binary alloys. The increase of Li, decrease the position at which the first maxima occurs for $\omega_L(q)$ and $\omega_T(q)$ .The influence of exchange and correlated motion of electron through various local–field correction functions raises the phonon modes than those due to static Hartree effect. The inclusion of local–field correction does not affect (by large amount) the position of the maxima, minima of longitudinal and transverse modes.

The position of the first minima coincides with the first peak in the structure factor of respective systems. We have not superimposed $S(q) \rightarrow q$ curve on PDC to avoid complication in the figures. The computer simulations and analytical calculations have demonstrated that this minimum arises from a process analogous to the Umklapp scattering in the crystalline solids. This sharp first maximum in the static structure factor acts like a smeared out reciprocal lattice vector.

The results of longitudinal phonon modes in lithium are more close to recent theoretical study due to pratap et al [27]. They have reported the phonon modes using the approach of Bhatia and Singh [28] with the addition of Born- Mayer core term in the direct interaction between the ions. Comparison with the INS and INX results [46-47] also supports present data very well. The results for sodium are also inline with the other theoretical study [27]. For binary alloy combination $Li_{0.61}Na_{0.39}$, the calculated results are compared with the MD simulation [25] and OF-AIMD results [26]. It is established that for the lower q values, both longitudinal and transverse branch of PDC agrees very well but at higher values they are much deviated, though once again the present result matches fairly well when compared with the theoretical results [27]. Here the unavailibilty of experimental or theoretical data for $Li_{0.5}Na_{0.5}$ restricts us to make comment, but it is established that as the mass of lithium increses phonon mode in both longitudinal and transverse branches increases.

4. Conclusions

We conclude that the PDC generated from HB approach reproduces satisfactorily general characteristics of dispersion curves. The well recognized model potential with more advanced Farid (F) and Sarkar-Sen (S) local field correction functions generate consistent results. The results of phonon frequencies of Li, $Li_{0.61}Na_{0.39}$ and Na for both longitudinal and transverse branch are in good agreement with available MD data in long and short wavelength region. It is also to be noted that the present results of $Li_{0.50}Na_{0.50}$ provides useful set of data for both branches. Hence, the present results confirms the applicability of the model potential in the aforesaid properties and supports the present approach for studying the phonon dynamics of non-crystalline $Li_{0.61}Na_{0.39}$ and $Li_{0.5}Na_{0.5}$ binary alloys.

The model potential depends on effective core radius is used here to describe the electron-ion interaction. Additional repulsive part outside the core vanishes faster than only Coulomb potential as $r \rightarrow \infty$ and hence represents the modification in the Ashcroft's empty core model. It may be noted that the inclusion of this repulsive term outside the core makes the effective core smaller than the ionic radius of a free ion.

The dispersion relations obtained for non-crystalline Li, $Li_{0.50}Na_{0.50}$, $Li_{0.69}Na_{0.31}$ and Na using the present theoretical approach derived from pair correlation function are quite satisfactory. Such study can also be carried out using local and non-local pseudopotential which will judge the success and applicability of the model pseudopotentials.

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