A 1  STRUCTURAL STUDY OF LIQUID RARE EARTH METALS FROM CHARGED HARD SPHERE REFERENCE FLUID 279
A 2  STRUCTURAL ANALYSIS OF LIQUID 3d TRANSITION METALS USING CHARGED HARD SPHERE REFERENCE SYSTEM 288
A 3  ELECTRONIC STRUCTURE AND PHONON DISPERSION RELATION OF LIQUID METALS 301

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• Though the CHS method [A1-A9] is proved very useful for explaining structural properties of liquid metals, the study of liquid rare earth metals using CHS is limited [A5].

• Gopala Rao and Bandyopadhyay [A5] have reported the structure factor $S(q)$, pair distribution function $g(r)$ and interatomic distance $r_i$ of nearest neighbour atoms for Nd, Dy, Ho, Er and Lu by employing CHS reference fluid with Ashcroft empty core model potential.

• They have fitted the input parameters like effective valency ($Z$), potential parameter ($r_c$) and hard sphere diameter ($\sigma$) in such a way that a good agreement with experimental findings to be obtained.

• The present appendix deals with the structural studies of some liquid rare earth metals, which reports the structure factor $S(q)$, pair distribution function $g(r)$ and interatomic distance $r_i$ of nearest neighbour atoms for liquid rare earth metals viz; Nd, Dy, Ho, Er and Lu by adopting Charged Hard Sphere (CHS) reference fluid.

• To describe electron–ion interaction, present model potential [A6-A12] along with the dielectric function due to Taylor [A13] is used.
• The important aspect of the present investigation is to make the computation free from any fitting procedure to reproduce correct experimental data, as it was done by Gopala Rao and Bandyopadhyay [A5].

• In the present investigations, the parameter of the potential is determined using [A14], \( r_c = 0.51(Z)^{\frac{1}{3}} R_a \), where \( R_a \) is the atomic radius.

• The constants and parameters used in the present computations are tabulated below Table (A 1.1).

**Table A 1.1: Parameters and constants used in present calculation**

<table>
<thead>
<tr>
<th>Metal</th>
<th>( T(K) )</th>
<th>( \rho (gm/cm^3) )</th>
<th>( Z )</th>
<th>( \eta )</th>
<th>( k_F (\AA^{-1}) )</th>
<th>( r_c (\AA) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nd</td>
<td>1473</td>
<td>6.78</td>
<td>1.5</td>
<td>0.40</td>
<td>1.0793</td>
<td>0.8113</td>
</tr>
<tr>
<td>Dy</td>
<td>1703</td>
<td>8.14</td>
<td>1.5</td>
<td>0.43</td>
<td>1.1025</td>
<td>0.7899</td>
</tr>
<tr>
<td>Ho</td>
<td>1753</td>
<td>8.25</td>
<td>1.5</td>
<td>0.43</td>
<td>1.1020</td>
<td>0.7868</td>
</tr>
<tr>
<td>Er</td>
<td>1793</td>
<td>8.37</td>
<td>1.5</td>
<td>0.44</td>
<td>1.1022</td>
<td>0.7828</td>
</tr>
<tr>
<td>Lu</td>
<td>1953</td>
<td>9.18</td>
<td>1.5</td>
<td>0.44</td>
<td>1.1197</td>
<td>0.7725</td>
</tr>
</tbody>
</table>

• The method for computing \( S(q) \), \( g(r) \) and \( r_t \) is given in Chapter 3.

• Figures (A 1.1)-(A 1.5) show the computed values of \( S(q) \) and \( g(r) \) of Nd, Dy, Ho, Er and Lu, respectively along with the experimental findings [A15].
Figure A 1.1: Structure factor, $S(q)$ and pair distribution function, $g(r)$ for Nd at 1473K
Figure A 1.2: Structure factor, $S(q)$ and pair distribution function, $g(r)$
for Dy at 1703K.
Figure A 1.3: Structure factor, $S(q)$ and pair distribution function, $g(r)$ for Ho at 1753K.
Figure A 1.4: Structure factor, $S(q)$ and pair distribution function, $g(r)$ for Er at 1793K
Figure A 1.5: Structure factor, $S(q)$ and pair distribution function, $g(r)$ for Lu at 1953K
• In Table (A 1.2), we have compared the position of the first and second peaks in $S(q)$ with experimental results of Waseda [A15].

Table A 1.2: Position of first and second peak in $S(q)$ ($\text{Å}^{-1}$) and interatomic distance ($r_1$) ($\text{Å}$)

<table>
<thead>
<tr>
<th>Metal</th>
<th>Peak positions in $S(q)$ ($\text{Å}^{-1}$)</th>
<th>Interatomic distance $r_1$ ($\text{Å}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nd</td>
<td>2.116</td>
<td>2.10</td>
</tr>
<tr>
<td>Dy</td>
<td>2.173</td>
<td>2.12</td>
</tr>
<tr>
<td>Ho</td>
<td>2.173</td>
<td>2.21</td>
</tr>
<tr>
<td>Er</td>
<td>2.173</td>
<td>2.24</td>
</tr>
<tr>
<td>Lu</td>
<td>2.210</td>
<td>2.28</td>
</tr>
</tbody>
</table>

• The deviation of presently generated results from experimental data at the first peaks of $S(q)$ are of the order of 0.16% to 0.27%. Similarly, for $g(r)$ these deviations are of the order of 0.52% to 0.74%.

• For all the five liquid rare earth metals the magnitude of the first peak in $S(q)$ and $g(r)$ are slightly higher than the experimental data, but the position of the first and second peaks in $S(q)$ are well estimated.

• The interatomic distance $r_1$ of the nearest neighbour atoms is also investigated and compared with other theoretical [A5] as well as experimental findings [A15] in Table 2. The excellent qualitative agreements between present and experimental findings are obtained.

• Gopala Rao and Bandyopadhyay [A5] have chosen valency ($Z$), potential parameter ($r_c$) and hard sphere diameter ($\sigma$) in such a way
that it yields satisfactory structural data. They have fitted these three parameters to obtain correct experimental predictions. While the present investigation is free from such kind of fitting procedure. In the previously reported study of liquid rare earth metals, the uncertainty in the data $Z$ is observed.

- Delley et al. [A16] have estimated $Z = 1.3$, Duthie and Pettifor [A17] have estimated the value $Z = 1.1$ to 1.5. Waseda and Miller [A18] have estimated $Z = 1.33$ to 2.09 for Lu. For Lu, Delley et al. [A16] has suggested $Z$ closer to two. While Johansson [A19] have assumed $Z = 3$.

- Gopala Rao and Bandyopadhyay [A5] have taken $Z = 1.54$ to 2.03 for obtaining better agreement with the experimental findings. So instead of making adjustment in $Z$, we have considered $Z = 1.5$ for all the five liquid rare earth metals and the uncertainty in the parameters are totally avoided, consistently.

- At the end we conclude that, though the present computation is free from any artificial fitting procedure to predict correct experimental data, it is capable of explaining very good results for the structural data of liquid rare earth metals.

- Hence the reported data are more meaningful and will provide better source for further comparison either with theoretical or experimental data.

- This confirms the applicability of our model potential and CHS method for predicting the structural studies of the liquid rare earth metals.
One of the most interesting points in the field of liquid state physics is whether the liquid structure of transition metals having the incomplete d shell differs from that of simple metals such as aluminum.

For this reason, the current appendix A 2 on the structural analysis of liquid 3d transition metals viz; Ti, V, Cr, Mn, Fe, Co, Ni and Cu are shown below.

Here we report the structure factor $S(q)$, pair distribution function $g(r)$, interatomic distance $r_i$ of nearest neighbour atoms and coordination number $n_i$ for liquid 3d transition metals using Charged Hard Sphere (CHS) reference system [A1-A9].

To describe electron–ion interaction, present model potential [A6-A12] along with the dielectric function due to Sarkar et al (SS) [A20] is used.

Here the potential parameter is estimated by employing the relation [A14], $r_c = 0.51(Z)^{-1/3} R_a$, where $R_a$ is the atomic radius.
The constants and parameters used in the present computations are tabulated below in Table (A 2.1).

Table A 2.1: Parameters and constants used in present computation

<table>
<thead>
<tr>
<th>Metal</th>
<th>$T(K)$</th>
<th>$\rho,(gm/cm^3)$</th>
<th>$Z$</th>
<th>$\eta$</th>
<th>$k_F,(\AA^{-1})$</th>
<th>$r_c,(\AA)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti</td>
<td>1973</td>
<td>4.15</td>
<td>1.5</td>
<td>0.44</td>
<td>0.3705</td>
<td>0.6461</td>
</tr>
<tr>
<td>V</td>
<td>2173</td>
<td>5.36</td>
<td>1.5</td>
<td>0.44</td>
<td>0.3954</td>
<td>0.6055</td>
</tr>
<tr>
<td>Cr</td>
<td>2173</td>
<td>6.27</td>
<td>1.5</td>
<td>0.45</td>
<td>0.4137</td>
<td>0.5787</td>
</tr>
<tr>
<td>Mn</td>
<td>1533</td>
<td>5.97</td>
<td>1.5</td>
<td>0.45</td>
<td>0.3995</td>
<td>0.5993</td>
</tr>
<tr>
<td>Fe</td>
<td>1823</td>
<td>7.01</td>
<td>1.5</td>
<td>0.44</td>
<td>0.4193</td>
<td>0.5710</td>
</tr>
<tr>
<td>Co</td>
<td>1823</td>
<td>7.70</td>
<td>1.5</td>
<td>0.45</td>
<td>0.4249</td>
<td>0.5634</td>
</tr>
<tr>
<td>Ni</td>
<td>1773</td>
<td>7.72</td>
<td>1.5</td>
<td>0.45</td>
<td>0.4258</td>
<td>0.5622</td>
</tr>
<tr>
<td>Cu</td>
<td>1423</td>
<td>7.97</td>
<td>1.5</td>
<td>0.46</td>
<td>0.4192</td>
<td>0.5711</td>
</tr>
</tbody>
</table>

- Figures (A 2.1)-(A 2.8) represent the generated $S(q)$ and $g(r)$ of Ti, V, Cr, Mn, Fe, Co, Ni and Cu, respectively, alongwith the experimental results [A15].
Figure A 2.1: Structure factor $S(q)$ and pair distribution function $g(r)$ for Ti at 1973K.
Figure A 2.2: Structure factor $S(q)$ and pair distribution function $g(r)$ for V at 2173K
Figure A 2.3: Structure factor $S(q)$ and pair distribution function $g(r)$ for Cr at 2173K
Figure A 2.4: Structure factor $S(q)$ and pair distribution function $g(r)$ for Mn at 1533K
Figure A 2.5: Structure factor $S(q)$ and pair distribution function $g(r)$
for Fe at 1823K
Figure A 2.6: Structure factor $S(q)$ and pair distribution function $g(r)$ for Co at 1823K.
Figure A 2.7: Structure factor $S(q)$ and pair distribution function $g(r)$ for Ni at 1773K
Figure A 2.8: Structure factor $S(q)$ and pair distribution function $g(r)$ for Cu at 1423K.
Table (A 2.2) and Table (A 2.3) represent the positions of first and second peak and related magnitude in $S(q)$ and $g(r)$, respectively.

**Table A 2.2:** Positions of First and Second Peak and related magnitude in $S(q)$

<table>
<thead>
<tr>
<th>Metal</th>
<th>First Peak position and Related magnitude in $S(q)$</th>
<th>Second Peak position and Related magnitude in $S(q)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Peak position $q_1$ (Å$^{-1}$)</td>
<td>Related magnitude</td>
</tr>
<tr>
<td>Ti</td>
<td>2.6334</td>
<td>2.45</td>
</tr>
<tr>
<td>V</td>
<td>2.8098</td>
<td>2.70</td>
</tr>
<tr>
<td>Cr</td>
<td>2.9040</td>
<td>3.00</td>
</tr>
<tr>
<td>Mn</td>
<td>2.8250</td>
<td>2.85</td>
</tr>
<tr>
<td>Fe</td>
<td>2.9800</td>
<td>2.95</td>
</tr>
<tr>
<td>Co</td>
<td>3.0202</td>
<td>3.00</td>
</tr>
<tr>
<td>Ni</td>
<td>3.0266</td>
<td>3.10</td>
</tr>
<tr>
<td>Cu</td>
<td>2.9644</td>
<td>3.00</td>
</tr>
</tbody>
</table>

**Table A 2.3:** Position of First and Second Peak and related magnitude in $g(r)$

<table>
<thead>
<tr>
<th>Metal</th>
<th>First Peak position and Related magnitude in $g(r)$</th>
<th>Second Peak position and Related magnitude in $g(r)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Peak position $r_1$ (Å)</td>
<td>Related magnitude</td>
</tr>
<tr>
<td>Ti</td>
<td>2.7993</td>
<td>3.20</td>
</tr>
<tr>
<td>V</td>
<td>2.6300</td>
<td>2.80</td>
</tr>
<tr>
<td>Cr</td>
<td>2.5400</td>
<td>2.50</td>
</tr>
<tr>
<td>Mn</td>
<td>2.6247</td>
<td>2.60</td>
</tr>
<tr>
<td>Fe</td>
<td>2.5083</td>
<td>2.60</td>
</tr>
<tr>
<td>Co</td>
<td>2.4818</td>
<td>2.50</td>
</tr>
<tr>
<td>Ni</td>
<td>2.4765</td>
<td>2.50</td>
</tr>
<tr>
<td>Cu</td>
<td>2.5294</td>
<td>2.50</td>
</tr>
</tbody>
</table>
• From Tables (A 2.2) and (A 2.3), it is found that the first and second peak position and related magnitude in $S(q)$ and $g(r)$ are in good agreement with the experimental data [A15].

• From the Figures (A 2.1) – (A 2.8), it is seen that as the atomic number increases from Ti to Cu, the oscillations of the structure factor systematically increase in amplitude.

• A noticeable discrepancy between present results and experimental data [A15] has been found in Ti and V. The results of $S(q)$ and $g(r)$ for rest of the 3d transition metals are in better agreement.

• From the careful analysis of the figures, it is found that a discrepancy between present results and experimental data [A15] go on decreasing as the atomic number increases from Ti to Cu. For Cu the excellent agreement has been obtained.

• This characteristic must be related to the incomplete 3d shell of these elements because the structural information obtained experimentally seems to be affected more or less by the electronic structure of outer shell for these elements.

• These results give qualitative support for the suggestion that a partial overlap of one atom with another for the elements having a nearly empty d shell such as Ti, is larger than that for the elements having a nearly filled d shell such as Ni. While in the case of Cu it is (d shell) fully filled up.

• This characteristic structure plays a significant role in a discussion of the excess entropy.
The interatomic distance $r_i$ of the nearest neighbour atoms and Coordination number $n_i$ are also calculated and represented alongwith the experimental data [A15] in Table (A 2.4).

Table A 2.4: Interatomic distance $r_i$ and Coordination number $n_i$

<table>
<thead>
<tr>
<th>Metal</th>
<th>Interatomic distance $r_i$ in (Å)</th>
<th>Coordination $n_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Present</td>
<td>Expt.</td>
</tr>
<tr>
<td>Ti</td>
<td>2.7993</td>
<td>3.20</td>
</tr>
<tr>
<td>V</td>
<td>2.6300</td>
<td>2.80</td>
</tr>
<tr>
<td>Cr</td>
<td>2.5400</td>
<td>2.50</td>
</tr>
<tr>
<td>Mn</td>
<td>2.6247</td>
<td>2.60</td>
</tr>
<tr>
<td>Fe</td>
<td>2.5083</td>
<td>2.60</td>
</tr>
<tr>
<td>Co</td>
<td>2.4818</td>
<td>2.50</td>
</tr>
<tr>
<td>Ni</td>
<td>2.4765</td>
<td>2.50</td>
</tr>
<tr>
<td>Cu</td>
<td>2.5294</td>
<td>2.50</td>
</tr>
</tbody>
</table>

Good agreements have been found between the present results and experimental data [A15] in both the cases i.e. interatomic distance $r_i$ and coordination number $n_i$.

The deviations from the experimental data [A15] in the case of coordination number $n_i$ are found highest 4.22% for Ti while lowest 0.31% for Cu.

In the past people have fitted valency ($Z$) in such a way that a good agreement with experimental findings is obtained. But in the present investigation we have considered $Z = 1.5$ instead of making adjustment in $Z$.

Lastly, we conclude that CHS reference system with our own model potential is capable to explain the structural information of liquid 3d transition metals, successfully.
A 3 ELECTRONIC STRUCTURE AND PHONON DISPERSION RELATION OF LIQUID METALS

• Present appendix A 3 deals with the computation of the electron and phonon dispersion curves of some liquid metals viz; Na (Z=1), Mg (Z=2), Al (Z=3) and Pb (Z=4) with the aim to explore the application of our newly constructed form of the pseudopotential [A6-A12].

• To describe the structural information we adopt here the Charged Hard Sphere (CHS) reference system [A1-A9].

• The choice of pseudopotential form factor is certainly an important consideration in the study of metallic properties and its actual form is much more sensitive to the choice of dielectric function of the electron gas. Hence, the purpose of present appendix is not only to generate the electron and phonon dispersion curve, but also to see the influence of various local-field correction functions in the screening. So we incorporated three different forms of the exchange and correlation functions, viz; Hartree (H) [A21], Taylor (T) [A13] and Sarkar et al (SS) [A20].

• The electronic structure of liquid metals using the pseudopotential theory and second-order perturbation theory is given as [A22-A24]

\[ E(k) = E_0(k) + E_1(k) + E_2(k), \]  
(A3.1)
where

\[ E_0(k) = \frac{\hbar^2 k^2}{2m}, \tag{A3.2} \]

\[ E_1(k) = N(k | W(q) | k), \tag{A3.3} \]

and

\[ E_2(k) = \frac{2m}{\hbar^2} \sum_q \frac{S(q) S^*(q) |W(q)|^2}{k^2 - |k + q|^2}, \tag{A3.4} \]

Using the structure factor \( S(q) \), equation (A3.1) becomes

\[ E(k) = \frac{\hbar^2 k^2}{2m} + \frac{2m}{\hbar^2} \left[ \sum_q \frac{S(q) |W(q)|^2}{k^2 - |k + q|^2} - \frac{S(q) |W(q)|^2}{q^2} \right], \tag{A3.5} \]

For liquid metals this equation is restructured as [A22-A24],

\[ E(k) = \frac{\hbar^2 k^2}{2m} + \Delta(k) - \Delta(0). \tag{A3.6} \]

Here

\[ \Delta(k) = \frac{3Z}{8k_F E_F k} \int_0^\infty S(q) W^2(q) q \ln \left| \frac{2k + q}{2k - q} \right| dq, \tag{A3.7} \]
and

$$\Delta(\theta)=\frac{3Z}{2k_F E_F} \int_{-\infty}^{\infty} S(q) W^2(q) dq. \quad (A3.8)$$

Hence the electron dispersion relation is derived as

$$\Delta E(k) = \Delta(k) - \Delta(\theta). \quad (A3.9)$$

To compute the phonon dispersion relations of liquid metals, the most frequently used approach of Hubbard and Beeby [A25] is adopted. With the physical argument that the product of the static pair correlation function $g(r)$ and the second derivative of the interatomic potential $\Phi(r)$ is peaked near the hard sphere diameter $\sigma$, Hubbard and Beeby [A25] have derived the expression for the longitudinal phonon frequencies $\omega_L(q)$ and the transverse phonon frequencies $\omega_T(q)$ as [A25, A26],

$$\omega_L^2(q) = \omega_E^2 \left[ 1 - \frac{3 \sin(q\sigma)}{(q\sigma)} - \frac{6 \cos(q\sigma)}{(q\sigma)^2} + \frac{6 \sin(q\sigma)}{(q\sigma)^3} \right] \quad (A3.10)$$

and

$$\omega_T^2(q) = \omega_E^2 \left[ 1 + \frac{3 \cos(q\sigma)}{(q\sigma)^2} - \frac{3 \sin(q\sigma)}{(q\sigma)^3} \right]. \quad (A3.11)$$

Here $\omega_E$ represents the maximum phonon frequency and is given as
\[ \omega_E = \frac{4\pi \rho \int_0^\infty g(r)r^2 \Phi''(r) \, dr}{3M} . \quad (A3.12) \]

With

\[ \Phi''(r) = \frac{4Z^2}{r^3} + \frac{\Omega}{\pi r^2} \int_0^\infty [F(q)q^2 \left( \frac{2\sin(qr)}{qr^3} - \frac{2\cos(qr)}{r^2} - \frac{q\sin(qr)}{r} \right)] \, dq, \quad (A3.13) \]

and

\[ g(r) = 1 + \frac{1}{2\pi^2 \rho r} \int_0^\infty \left( S(q) - 1 \right) q \sin(qr) \, dq. \quad (A3.14) \]

Here \( \rho, M, g(r), \Omega, F(q) \) and \( S(q) \) be the number density, atomic mass, pair correlation function, atomic volume, energy wave number characteristic and the structure factor of the element, respectively.

- The constants and parameters used in the present computations are tabulated below in Table (A 3.1).

**Table A 3.1:** Parameters and constants used in present computation

<table>
<thead>
<tr>
<th>Metal</th>
<th>( T(K) )</th>
<th>( \rho (gm/cm^3) )</th>
<th>( Z )</th>
<th>( \eta )</th>
<th>( k_F (\AA^{-1}) )</th>
<th>( r_e (\AA) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na</td>
<td>378</td>
<td>0.928</td>
<td>1</td>
<td>0.46</td>
<td>0.2509</td>
<td>0.7650</td>
</tr>
<tr>
<td>Mg</td>
<td>953</td>
<td>1.545</td>
<td>2</td>
<td>0.46</td>
<td>0.3675</td>
<td>0.6167</td>
</tr>
<tr>
<td>Al</td>
<td>943</td>
<td>2.37</td>
<td>3</td>
<td>0.45</td>
<td>0.4690</td>
<td>0.5278</td>
</tr>
<tr>
<td>Pb</td>
<td>613</td>
<td>10.66</td>
<td>4</td>
<td>0.46</td>
<td>0.4318</td>
<td>0.5186</td>
</tr>
</tbody>
</table>
• The attempts of studying the electronic structure and phonon dispersion curves of liquid metals using the pseudopotential theory are very rare and not exhaustive [A22-A24]. Srivastava [A22] and Gajjar et al [A24] have reported the electron dispersion of some simple liquid metals.

• For liquid metals, it was observed that there exists a deviation in the electron dispersion from the free electron value. It was also found that the maximum deviation takes place in the vicinity of the first spherical Brillouin zone. This region lies nearly at half of the distance of the first peak in the structure factor.

• The computed electron dispersions are shown in Figures (A 3.1) - (A 3.2) for liquid metals viz; Na (Z=1), Mg (Z=2), Al (Z=3) and Pb (Z=4).
Figure A 3.1: Electron dispersion curves for liquid Na and Mg
Figure A 3.2: Electron dispersion curves for liquid Al and Pb
It is evident from Figures (A 3.1) - (A 3.2) that

- The effect of various local-field correction functions is clearly visible for higher values of wave vector.

- The depth of the negative humps in the electron dispersion of liquid metals increases in the order of Na, Mg, Al and Pb.

- This gives the clear demonstration of the fact that the strength of the potential increases as we move from $Z = 1$ to $Z = 4$.

- The oscillatory behaviour in Figures (A 3.1) - (A 3.2) indicates that electron dispersion may have an important effect on the electronic properties of liquid metals.

The presently computed phonon dispersions for monovalent, divalent, trivalent and tetravalent liquid metals are shown in Figures (A 3.3) - (A 3.4).
Figure A 3.3: Phonon dispersion curves for liquid Na and Mg

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Figure A 3.4: Phonon dispersion curves for liquid Al and Pb
Here also it may be seen from Figures (A 3.3) - (A 3.4) that

- The dispersion of the longitudinal phonon exhibits oscillatory behaviour extending to the large wave vector transfer region.

- While in the case of transverse phonon, the oscillatory behaviour seems quite insignificant for high $q$ value.

- This indicates that the transverse phonon undergoes large thermal modulation than does the longitudinal phonon, due to the anharmonicity of atomic vibrations, which may be connected with the instability of transverse phonons in liquids.

- The $\omega \rightarrow q$ curves for transverse phonons attain maxima at a high $q$ value than the longitudinal phonon curve.

- 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 the position of the maxima, minima and the crossing of $\omega_c$ and $\omega_T$ modes, very significantly.

- The position of the first minima roughly coincides with the first peak in the structure factor of respective systems. 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.

In our literature survey we have found the experimental phonon frequencies only for liquid Na [A27] and Al [A28].

- The comparison of presently computed result for liquid Na with experimental results [A27] is highly encouraging. As the experimental results [A28] for Al are only few in numbers, a conclusive comparison with the presently calculated results is not made.

- Finally, we conclude that our model potential alongwith CHS reference system is capable to explain the electronic structure and phonon dispersion relation for monovalent, divalent, trivalent and tetravalent liquid metals.
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