

DIFFERENT REFERENCE SYSTEMS IN THE STUDY OF STRUCTURAL PROPERTIES OF SOME SIMPLE LIQUID METALS

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In the present paper three reference systems: Percus–Yevick hard sphere (PYHS), one component plasma (OCP) and charged hard sphere (CHS) are employed to investigate the temperature-dependent structural properties of some simple liquid metals. The structure factor $S(q)$, pair-distribution function $g(r)$ and interatomic distance r_1 of nearest neighbour atoms for Mg, Zn, Al, In, Tl and Pb are reported. Our own model potential is employed along with the local field correction due to Sarkar et al. (SS) to describe electron-ion interaction. It is seen that the CHS method alongwith the present form of model potential can explain more accurately the structural behaviour than PYHS and OCP methods.

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1. Introduction

During the last few decades, there has been an interest in the investigation of structural properties of liquid metals using different models as reference systems. Percus–Yevick hard sphere (PYHS) [1–4], one component plasma (OCP) [5–20], charged hard sphere (CHS) [21–27], hard sphere Yukawa (HSY) [28,29], soft sphere (SS) [30–32] and optimized random phase approximation (ORPA) [33–

36] are some of them. Looking to all earlier attempts and inferences [1–36], in the present paper three reference systems, i.e. PYHS, OCP and CHS, are employed to investigate the structural properties of some simple liquid metals viz. Mg, Zn, Al, In, Tl and Pb. The structure factor is one of the important properties to study the various electronic, magnetic, static and dynamic properties of material in liquid states. Therefore, one has to know very precisely the arrangement of atoms and ions. For this reason, the knowledge of the structure factor is the most essential part. The structure factor is a measure of particle correlations in the reciprocal space, and from the graphical presentation one can answer the question, what structural feature changes as material passes through a transition. Hence, accurate knowledge of this quantity is vital for studying numerous properties of liquid metals. The structure of liquid metals can be easily understood with the help of the model of a mixture of hard spheres. It is also possible to study the structure of a liquid metal in terms of the electron-electron, electron-ion and ion-ion structure factors by treating the liquid metal as a two-component, i.e. ion and electron fluid based on the perturbation theory employing pseudopotential.

The description of the atomic distribution in non-crystalline materials frequently employs the concept of the distribution function. In particular, the pair-distribution function $g(r)$, which corresponds to the probability of finding another atom at a distance r from the origin atom (at the point $r = 0$) is used. Since the pair-distribution function is obtained from diffraction data, this experimental information plays a significant role in the discussion of the structure and properties of non-crystalline materials. In addition, the concept of the distribution function can be extended to the crystal state as well as to multicomponent non-crystalline systems, imperfect gases and quantum fluids. $g(r)$ is frequently used for discussion of non-crystalline systems. The information given by $g(r)$ is only one-dimensional, but it does give quantitative information on the non-crystalline systems. Therefore, $g(r)$ is one of the most important pieces of information in the study of non-crystalline materials. It is a measure of pair correlation in the real space. From $g(r)$, some really fine features about the liquid metals can be made quite plausible on the basis of interaction forces.

To incorporate the electron-ion interaction, our well established model pseudopotential is used. The form of the model potential in real space is [25–27, 37–40]

$$W_B = \begin{cases} 0, & r < r_c, \\ -\frac{Ze^2}{r} [1 - \exp\{-r/r_c\}], & r \geq r_c. \end{cases} \quad (1)$$

This model potential is continuous in \mathbf{r} space and it is the modified version of the Ashcroft's empty core model [1]. In comparison with the Ashcroft empty core model potential [1], we have introduced $(Ze^2/r) \exp\{-r/r_c\}$ as a repulsive part outside the core which vanishes faster than the Coulomb potential $-Ze^2/r$ as $r \rightarrow \infty$. The

corresponding form factor in the reciprocal space is [25–27,37–40]

$$W_B(q) = \frac{-4\pi Ze^2}{\Omega q^2} \left[\cos(qr_c) - \frac{qr_c \exp\{-1\}}{1 + q^2 r_c^2} [\sin(qr_c) + qr_c \cos(qr_c)] \right]. \quad (2)$$

Here Z , e , Ω , q and r_c are the valency, electronic charge, atomic volume, wave vector and the parameter of the potential, respectively. In the present investigations, the parameter of the potential is determined by employing values of the wave vector, q_0 , where the form factor takes first zero value, i.e. $W_B(q) = 0$ for $q = q_0$. For the present model potential, the condition is $q_0 r_c = 1.3439$ [37,39,40].

2. Theory

The hard-sphere reference system is largely justified because it provides analytical representation in terms of a single parameter, σ , known as hard-sphere diameter, and reproduces the basic profile of the structure of liquid metals.

The structure factor $S_{\text{PYHS}}(q)$ due to the PYHS model is given by [1]

$$S_{\text{PYHS}}(q) = \left[1 + \frac{24\eta}{(1-\eta)^4 y^6} \left((1+2\eta)^2 y^3 (\sin y - y \cos y) \right. \right. \quad (3)$$

$$\left. \left. - 6\eta \left(1 + \frac{\eta}{2}\right)^2 y^2 [2y \sin y - (y^2 - 2) \cos y - 2] \right. \right.$$

$$\left. \left. + \frac{\eta}{2} (1+2\eta)^2 [(4y^3 - 24y) \sin y - (y^4 - 12y^2 + 24) \cos y + 24] \right) \right]^{-1},$$

with $y = q\sigma$.

The OCP reference system is an idealized system of pointlike charges moving in a neutralizing uniform background of opposite charges. An equilibrium state of the OCP system with the number density ρ and the temperature T may be characterized by a dimensionless plasma parameter $\Gamma = (Ze)^2 / (ak_B T)$, which measures the ratio between the average potential energy and the average kinetic energy per particle, where Ze is the charge of an ion and $a = [3/(4\pi\rho)]^{1/3}$ represents the ion-sphere radius whose volume equals the volume per electron.

If the assumption is made that the ionic liquid and the electron gas are weakly coupled to each other through pseudopotential as in the liquid metals, the electron gas screening can be taken into account by employing the random phase approximation. In the OCP scheme, the structure factor $S_{\text{OCP}}(q)$ is given by [20,27]

$$S_{\text{OCP}}(q) = \frac{S_0^{\text{OCP}}(q)}{1 + \rho\beta u^*(q)S_0^{\text{OCP}}(q)}. \quad (4)$$

In Eq. (4), $\rho = 1/\Omega$ is the number density, $\beta = 1/(k_B T)$, where k_B and T are the Boltzman constant and temperature of the system, respectively. $S_0^{\text{OCP}}(q)$ is the

static structure factor of the bare OCP reference system and the simple analytical expression of $S_0^{\text{OCP}}(q)$ is obtained as [20,27]

$$S_0^{\text{OCP}}(q) = \frac{1}{1 - \rho C_0^{\text{OCP}}(q)}, \quad (5)$$

with

$$\rho C_0^{\text{OCP}}(q) = \frac{3\Gamma}{q^4 a^4 \alpha_2^2} \left[\cos(qa\alpha_1) + 2 \cos(qa\alpha_2) - \frac{3 \sin(qa\alpha_1)}{qa\alpha_1} \right], \quad (6)$$

where α_1 and α_2 are dimensionless parameters given by

$$\alpha_1 = \begin{cases} -0.1455 \times 10^{-2}\Gamma + 0.9574 & (Z = 1), \\ -0.1455 \times 10^{-2}\Gamma + 1.0 & (Z = 2), \\ -0.1455 \times 10^{-2}\Gamma + 1.08 & (Z = 3), \\ -0.1455 \times 10^{-2}\Gamma + 1.15 & (Z = 4), \end{cases}$$

$$\alpha_2 = \begin{cases} 1.45 & (Z = 1), \\ 1.80 & (Z = 2), \\ 2.10 & (Z = 3), \\ 2.25 & (Z = 4). \end{cases} \quad (7)$$

$u^*(q)$ is the Fourier transform of the perturbative potential $u^*(r)$, which can be considered as the difference between the true interionic potential $u(r)$ and the OCP reference potential $a\Gamma/(\beta r)$. Thus the perturbation can be written in q space as

$$u^*(q) = \frac{4\pi Z^2 e^2}{q^2} [1 - F_N(q)] - \frac{4\pi a\Gamma}{\beta q^2}. \quad (8)$$

Here, $F_N(q)$ is the normalized-energy wave-number characteristic of the form

$$F_N(q) = \left(\frac{q^2}{4\pi Z e^2} \right)^2 \left(1 - \frac{1}{\varepsilon(q)} \right) \frac{1}{1 - f(q)} |W_B(q)|^2, \quad (9)$$

where $W_B(q)$ is the bare-ion pseudopotential and $\varepsilon(q)$ the modified dielectric function. In the present case, it includes exchange and correlation effects in the screening through local field correction function $f(q)$ due to Sarkar et al. [41].

The CHS reference system is essentially made up of positively charged identical hard spheres interacting via Coulomb potential embedded in a non-responding background of conduction electrons. The positively-charged hard spheres are assumed to occupy certain finite dimension in space. This system has been solved exactly by Palmer and Weeks [21] within a mean spherical approximation inside the core and outside the core, where a perturbation in the form of Coulomb interaction is assumed to act.

Within a linear screening approximation, the static structure factor $S_{\text{CHS}}(q)$ of a liquid metal under CHS reference system is given by [21,23 – 27]

$$S_{\text{CHS}}(q) = \frac{S_0^{\text{CHS}}(q)}{1 + \rho\beta\bar{V}(q)S_0^{\text{CHS}}(q)}. \quad (10)$$

Here, $S_0^{\text{CHS}}(q)$ is the static structure factor of the CHS reference system. The simple analytical expression of $S_0^{\text{CHS}}(q)$ is obtained as

$$S_0^{\text{CHS}}(q) = \frac{1}{1 - \rho C_0^{\text{CHS}}(q)}, \quad (11)$$

with

$$\begin{aligned} \rho C_0^{\text{CHS}}(q) = & \frac{24\eta}{y^6} [Ay^3(\sin y - y \cos y) + By^2(2y \sin y - (y^2 - 2) \cos y - 2) \\ & + Cy((3y^2 - 6) \sin y - (y^2 - 6)y \cos y) + D((4y^2 - 24)y \sin y \\ & - (y^4 - 12y^2 + 24) \cos y + 24) + \frac{E}{y^2}(6(y^4 - 20y^2 + 120)y \sin y \\ & - (y^6 - 30y^4 + 360y^2 - 720) \cos y - 720)], \end{aligned} \quad (12)$$

with $y = q\sigma$. The coefficients in Eq. (12) are given by

$$\begin{aligned} A &= -\frac{(1+2\eta)^2}{(1-\eta)^4} + \frac{Q^2}{4(1-\eta)^2} - \frac{(1+\eta)Qk}{12\eta} - \frac{(5+\eta^2)k^2}{60\eta}, \quad B = 6\eta M^2, \\ C &= \frac{k^2}{6}, \quad D = \frac{\eta}{2}(A + k^2U), \quad E = \frac{\eta k^2}{60}, \quad \gamma = \beta \frac{(Ze)^2}{\varepsilon_0\sigma}. \end{aligned}$$

Here σ is the effective hard-core diameter of the charged spheres and is the ion-ion coupling strength, $\beta = 1/(k_{\text{B}}T)$, k_{B} is the Boltzmann constant, T is the absolute temperature of the system, Ze is the ionic charge and ε_0 is the static dielectric constant of the system. Since the electron background is uniform, its dielectric constant is unity. $\eta = (\pi/6)\rho\sigma^3$ is the packing fraction and $k = (24\eta\gamma)^{1/2}$ gives the inverse screening length due to Debye and Hückel, and

$$\begin{aligned} Q &= \frac{1+2\eta}{1-\eta} \left[1 - \left(1 + \frac{2(1-\eta)^3k}{(1+2\eta)^2} \right)^{1/2} \right], \\ M &= \frac{Q^2}{24\eta} - \frac{1 + \frac{1}{2}\eta}{(1-\eta)^2}, \quad U = -\frac{1+\eta - \frac{\eta^2}{5}}{12\eta} - \frac{(1-\eta)Q}{12\eta k}. \end{aligned}$$

In Eq. (10), $\bar{V}(q)$ is the attractive screening correlation to the direct ion-ion potential of the form

$$\bar{V}(q) = \frac{W_{\text{B}}^2(q)}{\phi(q)} \left(\frac{1}{\varepsilon(q)} - 1 \right), \quad (13)$$

where $\phi(q) = 4\pi e^2/q^2$ is the Fourier transform of bare Coulombic interaction between two electrons. $\varepsilon(q) = 1 + [\varepsilon_H(q) - 1][1 - f(q)]$ is the modified dielectric function. It includes exchange and correlation effect in the screening through local field correction function $f(q)$. The function $\varepsilon_H(q)$ is called the static Hartree dielectric function for free electrons of the form

$$\varepsilon_H(q) = 1 + \frac{me^2}{2\pi k_F \hbar^2 Y^2} \left(\frac{1 - Y^2}{2Y} \ln \left| \frac{1 + Y}{1 - Y} \right| + 1 \right), \quad Y = \frac{q}{k_F}, \quad \hbar = \frac{h}{2\pi},$$

where m , k_F and h are the ionic mass, Fermi wave vector and Planck's constant, respectively. $\varepsilon_H(q)$ is time independent dielectric function and depends only on the magnitude of \mathbf{q} . Also it does not include any kind of exchange and correlation effects.

By taking Fourier transform of the structure factor, the pair distribution function $g(r)$ for the respective reference systems can be obtained by [24 – 27]

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

where $S(q)$ stands for one of the three different structure factors, i.e. $S_{\text{PYHS}}(q)$, $S_{\text{OCP}}(q)$ or $S_{\text{CHS}}(q)$.

3. Results and discussion

In present paper an attempt has being made to perform a detailed study of the structural properties of some simple liquid metals: Mg, Zn, Al, In, Tl and Pb at different temperatures. To incorporate temperature dependence in the present study, the following relation between temperature and packing fraction is used [42]

$$\eta(T) = A \exp\{-BT\}. \quad (15)$$

Where T is the absolute temperature and the parameters A and B are listed in Waseda [42].

It is also found that as temperature changes, the number density also changes. As the number density varies with the temperature, the Fermi wave vector k_F also varies and ultimately the potential parameter r_c (which is the function of k_F) is also affected by the temperature. Thus strength of the interatomic potential is also made temperature dependent.

The input parameters used to investigate the temperature dependence of the structural properties of liquid metals are tabulated in Table 1. The input parameters like Ω , k_F , η have been taken from Waseda [42] while the values of $q_0/(2k_F)$ are standard as listed in V. Heine et al. [43]. The plasma parameters Γ have been chosen in such a way that the results due to the OCP reference system are obtained in a good agreement with the experimental results [42].

TABLE 1. Input parameters and constants used to study temperature dependence.

Metal	T [K]	$q_0/(2k_F)$	r_c [Å]	Ω [Å ³]	k_F [Å ⁻¹]	η	Γ
Mg	953	0.83	0.6325	26.1096	0.3675	0.4522	120.00
	1063		0.6469	28.1690	0.3584	0.4363	100.00
	1153		0.4544	30.1204	0.3504	0.4237	90.00
Zn	723	0.95	0.4566	15.6985	0.4358	0.4534	120.00
	833		0.4587	15.9235	0.4337	0.4410	100.00
	933		0.5278	16.1550	0.4318	0.4300	90.00
Al	943	0.76	0.5293	18.9393	0.4690	0.4432	100.00
	1023		0.5355	19.0839	0.4676	0.4311	90.00
	1323		0.5140	19.7238	0.4623	0.3889	80.00
In	433	0.88	0.5169	27.1002	0.4158	0.4470	100.00
	573		0.5206	27.5482	0.4136	0.4286	90.00
	773		0.5248	28.1690	0.4106	0.4036	80.00
	973		0.5205	28.8184	0.4074	0.3801	70.00
Tl	588	0.90	0.5224	30.1204	0.4016	0.4519	100.00
	673		0.5246	30.3951	0.4001	0.4377	90.00
	773		0.5281	30.8642	0.3984	0.4217	80.00
	923		0.5316	31.4465	0.3958	0.3986	70.00
	1073		0.5186	32.0512	0.3932	0.3769	65.00
Pb	613	0.84	0.5229	32.2580	0.4318	0.4540	85.00
	823		0.5271	33.1125	0.4283	0.4071	70.00
	1023		0.5320	33.8983	0.4249	0.3669	65.00
	1173		0.6325	34.8432	0.4209	0.3395	60.00

The temperature dependent structure factors and pair distribution functions for the liquid metals under consideration are plotted in Figs. 1–6 and 7–12, respectively.

Tables 2 and 3 represent the first-peak positions and second-peak positions and related magnitudes for structure factor $S(q)$ along with experimental values [42].

Tables 4 and 5 represent the first-peak positions and second-peak positions and corresponding magnitudes for pair distribution function $g(r)$ along with experimental values [42]. The first-peak position represents the inter-atomic distance r_1 of the first nearest neighbor atoms, which corresponds to the first maxima of the $g(r)$ curve.

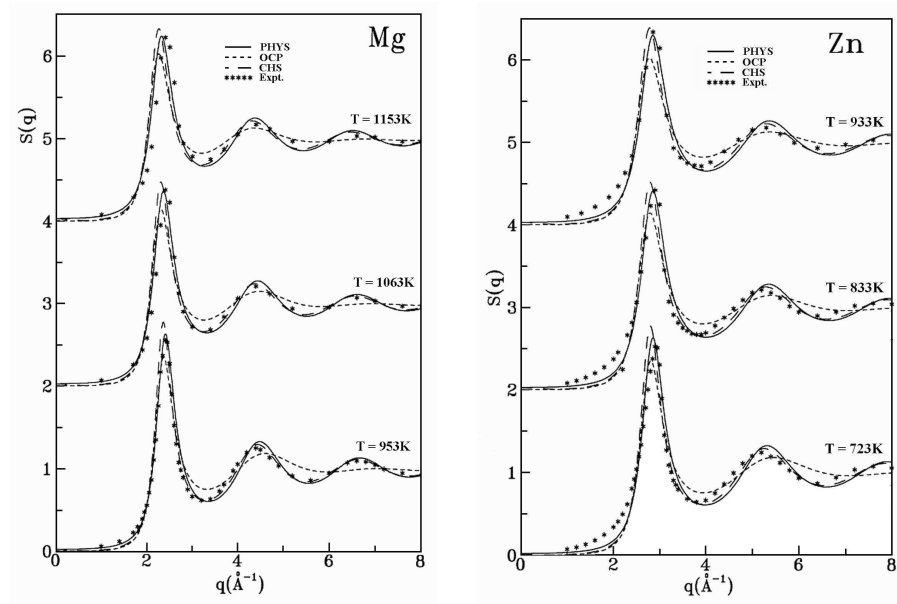


Fig. 1 (left). Temperature dependent structure factor $S(q)$ of liquid Mg.

Fig. 2. Temperature dependent structure factor $S(q)$ of liquid Zn.

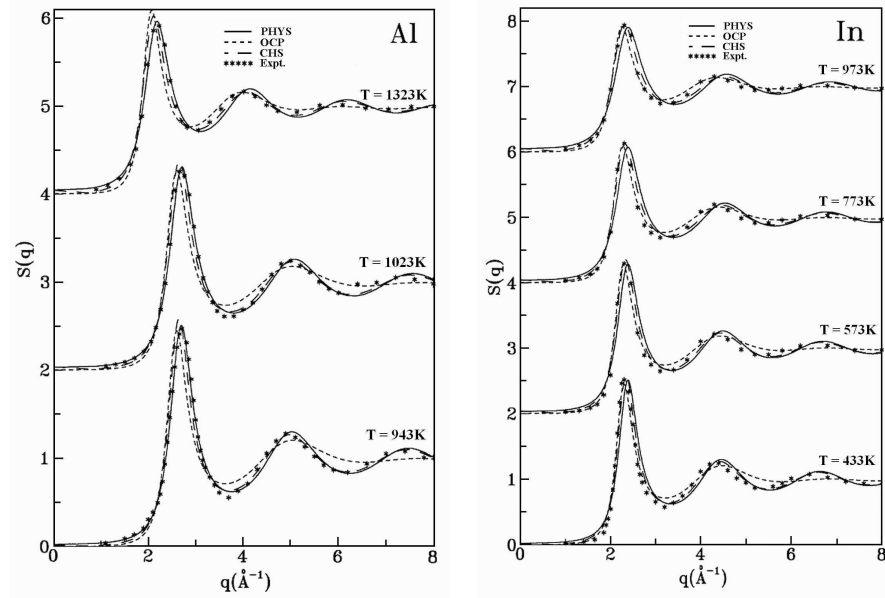


Fig. 3 (left). Temperature dependent structure factor $S(q)$ of liquid Al.

Fig. 4. Temperature dependent structure factor $S(q)$ of liquid In.

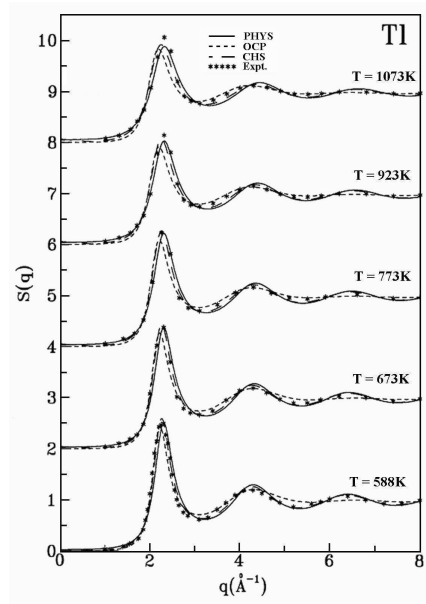


Fig. 5 (left). Temperature dependent structure factor $S(q)$ of liquid Tl.

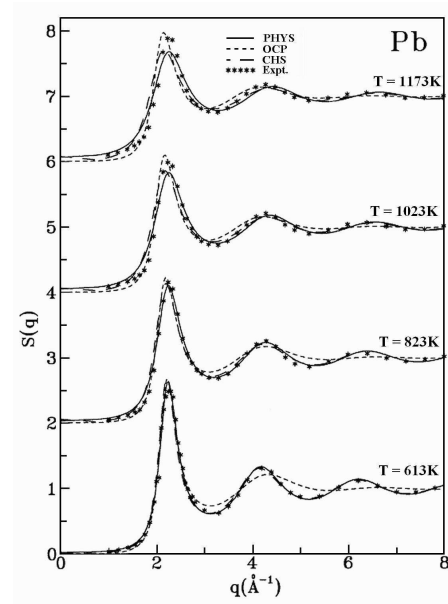


Fig. 6. Temperature dependent structure factor $S(q)$ of liquid Pb.

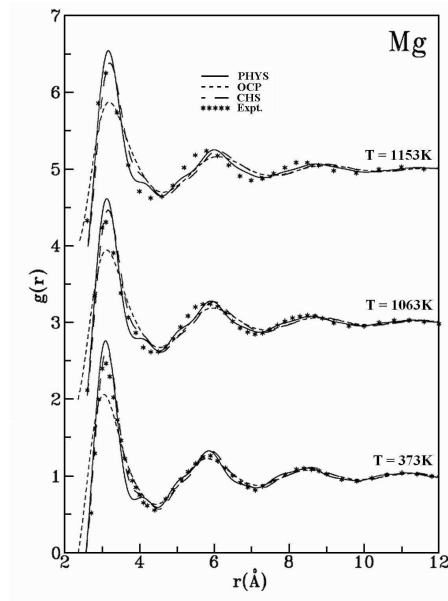


Fig. 7 (left). Temperature dependent pair-distribution function $g(r)$ of liquid Mg.

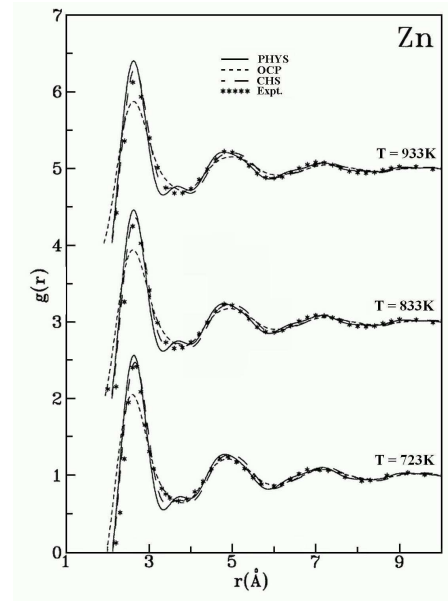


Fig. 8. Temperature dependent pair-distribution function $g(r)$ of liquid Zn.

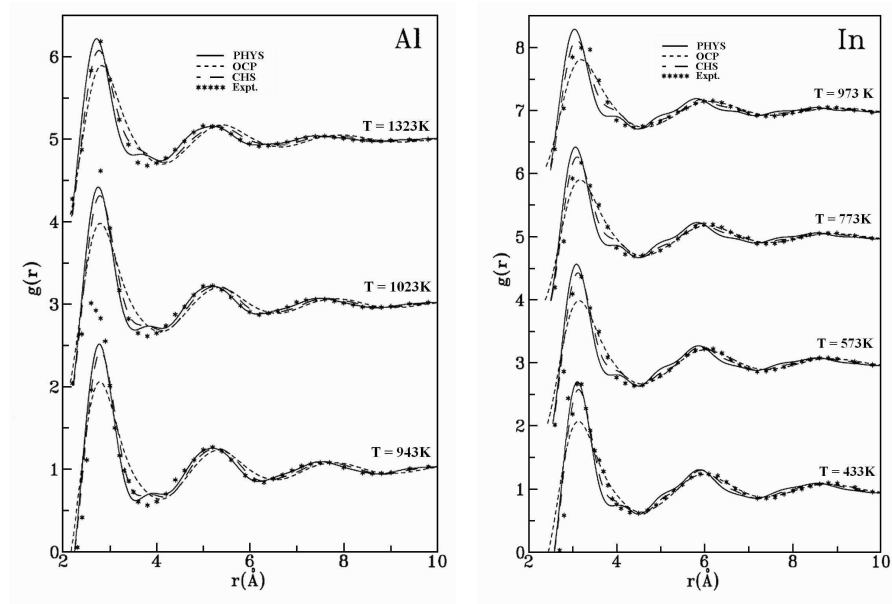


Fig. 9 (left). Temperature dependent pair-distribution function $g(r)$ of liquid Al.

Fig. 10. Temperature dependent pair-distribution function $g(r)$ of liquid In.

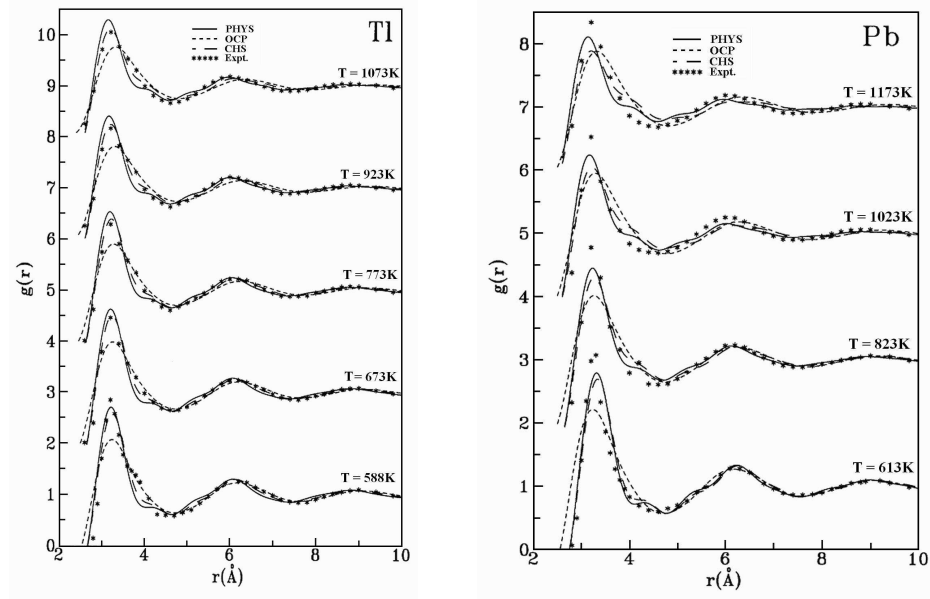


Fig. 11 (left). Temperature dependent pair-distribution function $g(r)$ of liquid Tl.

Fig. 12. Temperature dependent pair-distribution function $g(r)$ of liquid Pb.

TABLE 2. First-peak position and related magnitude in $S(q)$.

Metal	T [K]	First-peak position and related magnitude in $S(q)$							
		Peak position q_1 in \AA^{-1}				Related magnitude			
		PYHS	OCP	CHS	Exp.	PYHS	OCP	CHS	Exp.
Mg	953	2.4152	2.3627	2.3627	2.40	2.6322	2.3508	2.7756	2.556
	1063	2.3551	2.3039	2.3167	2.40	2.3651	2.1481	2.4751	2.381
	1153	2.3149	2.2524	2.2649	2.40	2.2445	2.0287	2.3369	2.223
Zn	723	2.8639	2.8016	2.3508	2.90	2.6322	2.3508	2.7756	2.527
	833	2.8497	2.8032	2.7878	2.90	2.4145	2.1481	2.5222	2.426
	933	2.8525	2.7754	2.7908	2.90	2.3034	2.0287	2.3937	2.375
Al	943	2.6969	2.5964	2.6466	2.70	2.5130	2.4512	2.5940	2.475
	1023	2.6890	2.5888	2.6389	2.70	2.3137	2.2729	2.3817	2.271
	1323	2.6912	2.5591	2.6086	2.70	1.9668	2.0947	2.0287	1.934
In	433	2.3912	2.3020	2.3466	2.30	2.5130	2.4513	2.5940	2.516
	573	2.3784	2.2897	2.3340	2.30	2.2892	2.2730	2.3582	2.297
	773	2.3904	2.2731	2.3171	2.30	2.0745	2.0947	2.1317	2.134
	973	2.3859	2.2550	2.2987	2.30	1.9084	1.9213	1.9531	1.939
Tl	588	2.3092	2.2232	2.2662	2.30	2.5130	2.4513	2.5941	2.499
	673	2.3007	2.2150	2.2579	2.30	2.3803	2.2730	2.4468	2.383
	773	2.3053	2.2057	2.2484	2.30	2.2260	2.0948	2.2792	2.240
	923	2.3040	2.1909	2.2333	2.30	2.0370	1.9213	2.0766	2.149
	1073	2.3030	2.1766	2.2328	2.30	1.8879	1.8375	1.9240	2.068
Pb	613	2.2515	2.2207	2.2207	2.30	2.6322	2.6688	2.6806	2.482
	823	2.2640	2.2028	2.2028	2.25	2.1017	2.2261	2.1315	2.150
	1023	2.2761	2.1851	2.1851	2.30	1.8271	2.0954	1.8547	1.987
	1173	2.2850	2.1648	2.1798	2.30	1.6816	1.9729	1.7092	1.894

It is seen that the structure factors and pair distribution function due to CHS method are in much better agreement with the experimental data in comparison with the PYHS and OCP.

From the pair distribution function $g(r)$, some really fine features about the liquid metals can be made available on the basis of inter-atomic forces. The van-

TABLE 3. Second-peak position and related magnitude in $S(q)$.

Metal	T [K]	Second-peak position and related magnitude in $S(q)$							
		Peak position q_2 in \AA^{-1}				Related magnitude			
		PYHS	OCP	CHS	Exp.	PYHS	OCP	CHS	Exp.
Mg	953	4.4891	4.6072	4.4366	4.40	1.3294	1.1866	1.2941	1.252
	1063	4.4414	4.4798	4.3774	4.40	1.2804	1.1521	1.2452	1.213
	1153	4.3671	4.3796	4.3171	4.40	1.2576	1.1348	1.2229	1.179
Zn	723	5.3232	5.4632	5.2609	5.20	1.3294	1.8668	1.2941	1.247
	833	5.3587	5.4362	5.2968	5.20	1.2894	1.1496	1.2548	1.220
	933	5.3659	5.3967	5.3196	5.20	1.2688	1.1018	1.2393	1.192
Al	943	5.0253	5.0588	4.9751	4.90	1.3076	1.2132	1.2767	1.286
	1023	5.0774	5.0273	5.0273	5.00	1.2707	1.1898	1.2394	1.253
	1323	5.1677	4.9696	5.0852	5.00	1.2044	1.1665	1.1704	1.171
In	433	4.4556	4.4853	4.4259	4.30	1.3076	1.2132	1.2767	1.263
	573	4.4909	4.4465	4.4465	4.30	1.2662	1.1898	1.2346	1.220
	773	4.5315	4.4142	4.4728	4.30	1.2253	1.1665	1.1928	1.204
	973	4.5828	4.3646	4.5101	4.30	1.1929	1.1435	1.1603	1.156
Tl	588	4.3029	4.3316	4.2599	4.20	1.3076	1.2132	1.2767	1.204
	673	4.3300	4.3014	4.2871	4.20	1.2830	1.1898	1.2525	1.201
	773	4.3545	4.2833	4.9760	4.30	1.2542	1.1665	1.2238	1.176
	923	4.3960	4.2405	4.3394	4.30	1.2180	1.1435	1.1874	1.160
	1073	4.4234	4.2128	4.3673	4.30	1.1888	1.1321	1.1573	1.132
Pb	613	4.1792	4.3334	4.1483	4.20	1.3294	1.2102	1.3042	1.307
	823	4.2834	4.2834	4.2528	4.30	1.2306	1.1683	1.2027	1.253
	1023	4.3853	4.2488	4.3246	4.30	1.1768	1.1547	1.1460	1.206
	1173	4.4499	4.2093	4.3597	4.30	1.1474	1.1412	1.1156	1.177

ishing of pair distribution function $g(r)$ at small values of r is due to the fact that as other atoms approach the central one closely, strong repulsive forces arise which push these atoms away. These repulsive forces, therefore, prevent the other atoms from the overlapping the central atom, which explains why $g(r) = 0$ at small values of r . The value of r where $g(r) = 0$ is nearly equal to the hard sphere diameter

TABLE 4. First-peak position and related magnitude in $g(r)$.

Metal	T [K]	First-peak position and related magnitude in $g(r)$							
		Peak position r_1 in Å				Related magnitude			
		PYHS	OCP	CHS	Exp.	PYHS	OCP	CHS	Exp.
Mg	953	3.0904	3.0480	3.1221	3.10	2.7593	2.0579	2.6577	2.463
	1063	3.1274	3.1221	3.1645	3.10	2.6162	1.9414	2.4652	2.308
	1153	3.1697	3.1909	3.2121	3.10	2.5424	1.8723	2.3814	2.249
Zn	723	2.6300	2.5876	2.6141	2.70	2.5619	2.0533	2.4464	2.418
	833	2.6194	2.6035	2.6511	2.60	2.4582	1.9409	2.3597	2.247
	933	2.6141	2.6141	2.6458	2.70	2.4015	1.8744	2.2983	2.134
Al	943	2.7729	2.7834	2.7993	2.80	2.5175	2.0603	2.4246	2.829
	1023	2.7515	2.7940	2.7834	2.80	2.4192	1.9799	2.3129	2.615
	1323	2.7146	2.8258	2.7623	2.80	2.2201	1.8930	2.0770	2.187
In	433	3.1115	3.1327	3.1380	3.10	2.6985	2.0687	2.5742	2.662
	573	3.0904	3.1486	3.1221	3.10	2.5665	1.9856	2.4273	2.397
	773	3.0692	3.1697	3.1062	3.20	2.4203	1.8978	2.2633	2.172
	973	3.0480	3.1962	3.0957	3.10	2.2903	1.8063	2.1186	2.025
Tl	588	3.2174	3.2385	3.2438	3.20	2.7004	2.0670	2.5747	2.746
	673	3.2015	3.2544	3.2332	3.20	2.6244	1.9845	2.4912	2.457
	773	3.1856	3.2650	3.2174	3.20	2.5306	1.8970	2.3862	2.285
	923	3.1592	3.2915	3.2965	3.20	2.4036	1.8059	2.2404	2.163
	1073	3.1380	3.3146	3.1856	3.20	2.2916	1.7594	2.1064	2.051
Pb	613	3.3126	3.2332	3.3338	3.30	2.7896	2.2131	2.6925	3.073
	823	3.2332	3.2597	3.2650	3.20	2.4491	2.1596	2.3055	2.776
	1023	3.1697	3.2862	3.2227	3.20	2.2418	1.9507	2.0493	2.525
	1173	3.1327	3.2179	3.2015	3.20	2.1139	1.8862	1.8701	2.342

of the atom. The major peak appearing in $g(r)$ is due to the fact that (except at very short distances) atoms attract each other, hence the force tends to pull other atoms towards the center, resulting in a particularly large density at certain specific distances. The damping oscillation in the curve of $g(r)$ arises from the interaction between the forces of central atom and near neighbours still farther away. For

TABLE 5. Second-peak position and related magnitude in $g(r)$.

Metal	T [K]	Second-peak position and related magnitude in $g(r)$							
		Peak position r_2 in Å				Related magnitude			
		PYHS	OCP	CHS	Exp.	PYHS	OCP	CHS	Exp.
Mg	953	5.8580	5.8157	5.9109	5.80	1.3273	1.2250	1.3252	1.264
	1063	5.9215	5.9639	5.9956	5.90	1.2794	1.1864	1.2695	1.241
	1153	6.0115	6.1015	6.1015	5.80	1.2517	1.1635	1.2390	1.238
Zn	723	4.8261	4.9002	4.9425	4.90	1.2723	1.2108	1.2694	1.238
	833	4.7996	4.9478	4.9531	4.90	1.2374	1.1743	1.2293	1.235
	933	4.7944	4.9849	4.9743	4.90	1.2175	1.1539	1.2075	1.232
Al	943	5.1912	5.3288	5.2865	5.20	1.2524	1.2296	1.2522	1.267
	1023	5.1860	5.3500	5.2971	5.10	1.2207	1.2032	1.2208	1.230
	1323	5.2018	5.4135	5.3500	5.10	1.1567	1.1759	1.1612	1.165
In	433	5.8898	5.9744	5.9374	6.00	1.3069	1.2320	1.2989	1.237
	573	5.8686	6.0062	5.9268	6.10	1.2686	1.2041	1.2562	1.225
	773	5.8474	6.0591	5.9215	6.10	1.2265	1.1755	1.2090	1.200
	973	5.8316	6.1173	5.9162	6.10	1.1898	1.1471	1.1678	1.152
Tl	588	6.0856	6.1861	6.1438	6.20	1.3020	1.2293	1.2951	1.256
	673	6.0697	6.2126	6.1491	6.10	1.2772	1.2023	1.2668	1.234
	773	6.0432	6.2443	6.1173	6.10	1.2472	1.1745	1.2325	1.218
	923	6.0009	6.2973	6.0909	6.00	1.2085	1.1486	1.1868	1.214
	1073	5.9639	6.3449	6.0856	6.00	1.1770	1.1331	1.1484	1.187
Pb	613	6.2337	6.1702	6.2708	6.20	1.3338	1.2726	1.3238	1.287
	823	6.1332	6.2285	6.2126	6.10	1.2211	1.2049	1.2030	1.238
	1023	6.0274	6.2867	6.1755	6.10	1.1582	1.1839	1.1286	1.257
	1173	5.9692	6.3502	6.1808	6.10	1.1262	1.1638	1.0876	1.189

the large values of r , the concentration approaches a constant value due to the short-range order of the liquid, the distribution of atoms is completely random and independent of position of central atom, i.e. independent of r , hence $g(r) \rightarrow 1$ as $r \rightarrow \infty$ is a situation corresponding to the absence of correlation between atoms.

In the study of the temperature dependent structural properties, some interesting results have been obtained. The main effect of the temperature variation is

the change in the amplitude of the oscillations in the structure factor and pair distribution function. Namely, a decrease around the peak and an increase elsewhere are observed. Also it is observed that at higher temperatures the first main peak tends to become flatter and broader with increasing temperature, but its position is usually unchanged. It is also found that the first- and second-peak positions of Zn are slightly greater than in other polyvalent metals (Mg, Al, In, Tl and Pb). This is due to the fact that the atomic volume of Zn is lower than of other polyvalent metals (Mg, Al, In, Tl and Pb).

From the comparison, it is seen that the CHS method along with the present form of model potential is able to explain more accurately the structural behaviour than PYHS and OCP methods. The discrepancy in the outcome of OCP with experimental observations [42] is found higher than those with CHS and PYHS. Thus the structure of polyvalent metals is better described by the PYHS and CHS than by the OCP reference system. Our study leads to the conclusion that CHS reference system is better than PYHS and OCP in explaining the structure of liquid metals. The results also confirm the use of our single-parametric model potential in explaining the structure of liquid metals.

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PROUČAVANJE STRUKTURNIH SVOJSTAVA NEKIH JEDNOSTAVNIH TEKUĆIH METALA U RAZLIČITIM REFERENTBIM SUSTAVIMA

Za istraživanje temperaturno-ovisnih svojstava strukture nekih jednostavnih tekućih metala, primijenili smo tri referentna sustava: Percus–Yevickov tvrde kugle, jednokomponentne plazme i nabijenih kuglica. Izvješćujemo o strukturnom faktoru $S(q)$, funkciji raspodjele parova $g(r)$ i o međuatomskim razmacima r_1 najbližih atoma u Mg, Zn, Al, In, Tl i Pb. Rabimo naš vlastiti modelski potencijal i popravku lokalnog polja prema Sarkaru i sur. za opis međudjelovanja elektron-ion. Nalazimo da metoda nabijene tvrde kuglice s primijenjenim modelskim potencijalom točnije opisuje strukturna svojstva nego druge dvije metode.