Computation of the Structure Factor of Some Transition Liquid Metals

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Abstract

Applying the solution of the Percus-Yevic equation to a one component hard sphere system and using the recently developed potential for liquid transition liquid metals, the structure factor of transition liquid metals were computed. The peak height and peak position of the structure factor of the liquid metals were studied. The results obtained were compared with available experimental values. The results obtained revealed that the structure factor of liquid transition metals computed using the harmer potential were in better agreement with experimental values and the use of the potential reproduced the structure factor, peak position and peak height of the structure factor of some transition liquid metals.

Keywords: liquid metals, structure factor, potential, peak position and peak height

1. Introduction

The liquid phase is a condensed phase of matter. The density of liquids is similar to those found in the corresponding solid phase but the symmetric of liquids is more typical of gases. At comparable temperatures, liquids have properties that are not very different from those of solids. Liquids exhibits a variety of properties comparable to that found in crystalline solids. The structure factor is one of the most important properties used to study various electronic, magnetic, dynamic equilibrium and thermodynamic properties of a material in the liquid state [1]. The structure factor is a measure of particle correlation in the reciprocal space [2]. Over the years, the study of liquid metals has attracted experimentalist, theoreticians and computational condensed matter physicists. The exact theories and experiments for some of the properties of liquid metals are still future problems. In the study of the structural properties of liquid metals, different inter-ionic potentials are developed and used. Khaleque et al; [3] used inter-ionic potential based on Bretonnet-Silbert formalism in combination with Faber-Ziman theory to calculate the partial statics structure factor of Ag-ln alloy. Effective pair potentials was used in conjunction with the thermodynamically self-consistent liquid theory and the variational modified hypernetted chain approximation to study the structural properties of liquid Ca, Sr and Bg. The results they obtained were in good agreement with experimental values [4]. The structural properties of face centred cubic metals transition metals (Cu, Ag, Au and Ni) near their melting points were calculated using the variational modified hypernetted chain theory with a new embedded atom method. The computed static factor and pair distribution function were in good agreement with the experimental values [5]. The structure factor of liquid metals was computed using the Stochy-hard-sphere potential. The computed structure factor of liquid metals was Fourier transformed to obtain the radial distribution function, they also determined the nearest neighbour distance, coordinator number and Ashcroft effective number of electrons per metallic atom of liquid metals. The structure factor of liquid metals they computed was in excellent agreement with experimental values [6]. The structure factor of liquid metals is determined experimentally using X-ray diffraction and neutron diffraction [7-12]. Different works on the structure factor of liquid metals have shown that an approach may give good results for a particular liquid metal or liquid metals that have similar characteristics [13-18].These may be due to

   i.   The type of potential used that may depend mainly on the electron density.
   ii.   The use of hand spheres interactions as initial approximation.
  iii.   The use of effective potential that depends on electron density as a real potential ion-ion interaction.

In this work, we use a recently developed potential to compute the structure factor of liquid transition metals and study the peak position and peak height in order to investigate the effectiveness of the potential in the computation and study of the properties of liquid metals.

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2. Theoretical considerations and computation

For a liquid system, the charged particles are present with oppositely charged background, which preserves the electrical neutrality. The system is a two component system with the following properties.

$$\ell_1 e_1 + \ell_2 e_2 = 1 \tag{1}$$

$$g_{12} = g_{21} = g_{22} = 1 \tag{2}$$

where ℓ is density, e is electronic charge, g_{ij} is the radial distribution function between species i and j. Subscript 1 is for the charged sphere while subscript 2 is for the background particles.

There is no correlation between the background particles, it sets the zero of energy of the system and does not directly affect the structure of the hand sphere fluid. This assumption reduces our system to a one component system such that

$\ell_1 = \ell_2$, $e_1 = e_2$ and $g = g_{ij}$.

Within the mean spherical approximation the mean spherical equation consists of the Ornstan-Zernike equation [19].

$$h(x) = C(x) + \ell d^3 \int h\left(|x - x'|\right) C(x') dx' \tag{3}$$

with the closure relation

$$h(x) = -1 \text{ or } g(x) = 0 \quad \text{for x<1}$$

$$C(x) = -\beta V(x) = -y/x \quad \text{for x>1}$$

where $\beta = \dfrac{1}{KT}$, $h(x) = g(x) - 1$ and $C(x)$ is the direct correlation function. For the solution of equation (3), we introduce the following dimensionless parameters.

$$x = \frac{r}{d}, \quad \eta = \frac{1}{6}\pi \ell d^3, \quad \gamma = \frac{\beta e^2}{d}, \quad k = (24\eta y)^{\frac{1}{2}} \tag{4}$$

where γ, k and η are the dimensionless variables which represent the ion-ion coupling strength, the Debye-Huckel inverse screening length and the packing fraction.

Equation (3) is solved for the C(x) in x<1 and for h(x) in x>1. The solution of equation (3) for the direct correlation function $C_0(x)$ is

$$C_0(x) = A + Bx + Cx^2 + Dx^3 + Ex^5 \tag{5}$$

where,

$$A = \frac{(1+2\Omega)^2}{(1-\eta)^4} + \frac{Q^2}{4(1-\eta)^2} - \frac{(1+\eta)QK}{12\eta} - \frac{(5+\eta^2)^2}{60\eta} \tag{6}$$

$$B = 6\eta M^2, \quad C = \frac{K^6}{6}, \quad D = \frac{\eta}{2}(A + K^2 U), \quad E = \frac{\eta K^2}{60} \tag{7}$$

and

$$Q = \frac{1+2\Omega}{1-\eta}\left[1 - \left(1 + \frac{2(1-\eta)^3 K}{(1+2\eta)^2}\right)^{\frac{1}{2}}\right] \tag{8}$$

$$M = \frac{Q^2}{24\eta} - \frac{1+0.5\eta}{1-\eta^2} \tag{9}$$

$$U = \frac{-(1+\eta-0.2\eta^2)}{12\eta} - \frac{(1-\eta)Q}{12\eta K} \tag{10}$$

The static structure factor is obtained by the Fourier transform, C(q) of the Ornstein-Zernike direct correlation function.

$$S(q) = \left[1 - \rho C_0(q)\right]^{-1} \tag{11}$$

Fourier transforming equation (5) gives [19].

$$\rho C_0 (q) = \frac{24\eta}{q^6} \begin{bmatrix} Aq^2 (\sin q - q \cos q) + Bq^2 \{2q \sin q - (q^2 - 2) \cos q - 2\} \\ +Cq\{(3q^2 - 6) \sin q - (q^2 - 6)\}q \cos q + \\ D\{(4q^2 - 24)q \sin q - (q^4 - 12q^2 + 24) \cos q + 24\} + \\ E\{6(q^4 - 20q^2 + 120)q \sin q - (q^6 - 30q^4 + \\ 360q^2 - 720) \cos q - 720\}/q^2 - \gamma q^4 \cos q \end{bmatrix} \tag{12}$$

In the long wavelength limit, equation (11) reduces to

$$\ln S_0(q) = \frac{q^2 \sigma^2}{24\eta\gamma} \left[1 + \frac{\alpha - 1}{24\eta\gamma} q^2 \sigma^2 \right] \tag{13}$$

where

$$\alpha = 24\eta \left[\frac{A}{3} + \frac{B}{4} + \frac{C}{5} + \frac{D}{6} + \frac{E}{8} + \frac{\gamma}{2} \right] \tag{14}$$

Within the linear screening approximation, the static structure factor of liquid metal is

$$S(q) = \frac{S_0(q)}{1 + \rho\beta V_{sc}(q) S_0(q)} \tag{15}$$

where

$$V_{sc} = \frac{V_B^2}{Q(q)} \left[\frac{1}{E(q)} - 1 \right] \tag{16}$$

Equation (16) is the screening correction to the direct ion-ion, potential $Q(q)$ is the Fourier transform of the bare Columbic interaction between two electrons, $E(q)$ is the wave vector dependent dielectric function. The dielectric function used is the modified Hartree dielectric function which gives good account of ionic correlation in metals. Also this dielectric function is well screened at small wave vector components and the dielectric function is

$$E(q) = \frac{4\pi m e^2 k_f}{\pi \hbar^2 q^2} \tag{17}$$

where m is electronic mass, e is charge of an electron, k_f is the Fermi wave, $Q(q)$ is the Fourier transform of the bare Coulomb interaction between two electrons given as

$$Q(q) = \frac{4\pi e^2}{q^2} \tag{18}$$

Based on the recently developed interatomic pair interaction in liquid transition metals, the interaction between the particles can be written as [20].

$$V(r) = B_1 \exp\left(-\frac{r}{q}\right) + B_2 \exp\left(-0.5\frac{r}{a}\right) \qquad r \leq Rc \tag{19}$$

$$V(r) = \frac{-Ze^2}{r} \qquad r \geq Rc \tag{20}$$

where

$$B_1 = \left(\frac{Ze^2}{R_c} \right) \left(1 - \frac{2a}{Rc} \right) \exp\left(\frac{Rc}{a} \right) \tag{21}$$

$$B_2 = \left(\frac{2Ze^2}{Rc} \right) \left(\frac{a}{Rc} - 1 \right) \exp\left(\frac{-0.5Rc}{a} \right) \tag{22}$$

where a=0.342a.u, Z is the valency, Rc is the Ashcroft core radius obtained from the stabilization condition [21] as

$$Rc = \left[\frac{2}{15} \left(\frac{9\pi}{4} \right)^{2/3} r_s + \frac{1}{6\pi} \left(\frac{9\pi}{4} \right)^{1/3} r_s^2 + \frac{1}{5} Z^{2/3} r_s^3 + \frac{2}{9} r_s^4 \frac{dE_c}{dr_s} \right] \tag{23}$$

where r_s is the electron gas parameter and E_c is the correlation energy. The correlation energy used in this work is given as [22].

$$E_c = \frac{-0.1423}{1 + 1.0529 r_s^{1/2} + 0.3339 r_s} \tag{24}$$

The bare ion form factor is the modified Ashcroft core Pseudopotential in reciprocal space given [21] as

$$V(q) = \frac{-4\pi Ze^2}{\Omega q^2}\left[\cos(qR_c) - \left\{\frac{qR_c\exp(-1)}{1+q^2R_c^2}\right\}(\sin qR_c) + qR_c\cos qR_c\right] \tag{25}$$

where Ω is the atomic volume and Rc is the Ashcroft core radius.

3. Result and discussion

The structure factor of liquid Fe obtained 1550k is shown in figure 1, while that of V is shown in figure 2. As revealed in the figures, there is good agreement between the experimental and the computed structure. The level of agreement between the computed structure factor and experimental value may be due to the potential used in the work. The potential is well screened in this case. Furthermore, the Ashcroft core radius, used in this work was computed and not fitted to obtain result that are in good agreement with experimental values. The first peak obtained is quite high compared with the second peak, revealing that the first peak is the most important characteristic feature of static structure factor of liquid metals. Also the peak position and peak heights are in good agreement with experimental values. The peak position occurs when the potential is a minimum which shows that the static structure factor of liquid metals are sensitive to the potential but not to its details [13].

Our results for the peak position of Zn and Cd are closer to experimental values than the ones obtained by Rao and Venkatesh that used the sticky-hand-sphere potential to compute the structure factor of liquid metals [6]. In the work of Dalgic et al., [5], the peak heights were over estimated as a result of the type of potential that used unlike the results we obtained. Our result for Cu, Ni, Au and Ag compares very well with the result Bhuiyan et al., [27]. But their work overestimated the peak heights although their peak positions were in good agreement with experimental values. The results obtained where is in better agreement with experimental values than the results obtained in our earlier work where the same type of potential was used to compute the structure factor of both simple and transition liquid metals and the results obtained for the transition liquid metals was poor [28].

Table 1 shows the first peak position and peak height of the structure factor of liquid metals. As shown in table 1, there is a good agreement between our computed peak position and peak height and available experimental values of some transition liquid metals. The little discrepancy between our result and experimental may be due to the densities of the liquid metals used in the computation and the one used for experimental studies as they may not be the same. The results obtained in this work compares very well with the result of Waseda [23] who studies the structure factor of transition liquid metals and their alloys theoretically.

4. Conclusion

The structure factor of some transition liquid metals has been studied successfully. The structure factor depends on the potential of the liquid metal studied. The Peak position of the structure factor of a liquid metal is an intrinsic property of the metal. The peak height is a function of some properties of the liquid metal such as temperature and density. The results obtained in this work for the structure factor, peak height, peak position of transition liquid metals is in very good agreement with experimental values which shows that the potential used in this work can be used to predict properties of transition metals to a reasonable level of accuracy.
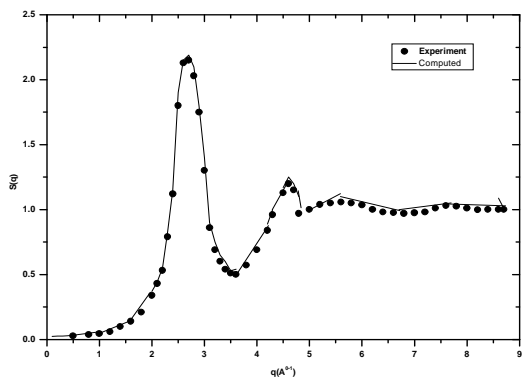

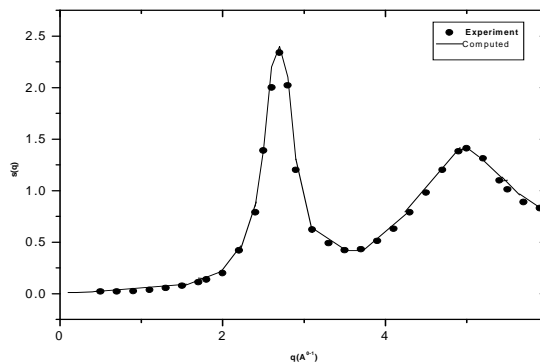Fig.1: Experimental and computed Structure factor of Fe at 1550K

Fig.2: Experimental and computed structure factor of liquid V at 1900K

Table 1: Computed and experimental peak position and peak height of some transition metals

Metal	R_s(a.u)	T(k)	Peak Position (Å)		Peak Height	
			Computed	Expt[23]	Computed	Expt[23 -26]
Zn	2.31	450	2.89	2.93	2.44	2.45
Cd	2.59	350	2.60	2.62	2.34	2.30
In	2.41	160	2.25	2.30	2.67	2.60
Tl	2.48	315	3.00	2.26	2.82	2.81
Cu	2.67	1150	2.90	3.00	2.60	2.50
Ag	3.02	1000	2.60	2.61	2.91	
Au	3.01	1150	2.64	2.66	3.25	
V	1.64	1900	2.70	2.71	2.48	2.47
Mn	2.14	1260	2.82	2.83	2.82	
Cr	1.86	1900	3.00	3.01	2.63	
Fe	2.12	1550	2.76	2.78	2.94	2.97
Co	2.07	1550	3.02	3.02	2.80	2.82
Ni	2.07	1550	3.09	3.10	3.15	3.20
Pd	2.28	1580	2.80	2.81	3.18	3.60

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