*Bangladesh Journal of Physics, Vol. **30**, Issue 1, pp. 23–34, June 2023*

ROLE OF INTERIONIOC INTERACTIONS ON THE SURFACE PROPERTIES OF LIQUIDS Zn, Sn AND Pb

NAWER BINTE ZOHA[1] and R. C. GOSH[2,*]

[1]*Department of Theoretical Physics, University of Dhaka, Dhaka-1000, Bangladesh*

[2]*Department of Physics, University of Dhaka, Dhaka-1000, Bangladesh*

**Corresponding author e-mail: ratan@du.ac.bd*

Received on 09.11.2022, Revised received on 15.02.2023, Accepted for publication on 16.02.2023.

DOI: ***https://doi.org/10.3329/bjphy.v30i1.79512***

ABSTRACT

Surface tension (γ) formula based on hard-sphere (HS) interaction developed from first and second order Percus-Yevick (PY) solutions for isothermal compressibility proposed by Mayer et al. has been used to calculate surface tension of liquid less simple metals Zn, Sn, and Pb. For calculation of surface entropy (S_v) of same metals, we have used the formula of Gosh et al. Effective HS diameter and corresponding packing fraction are key components of the employed HS theories. These components are calculated by utilizing Bretonnet-Silbert (BS) pseudopotential for interactions in metals and the Linearized Week-Chandler-Andersen (LWCA) theory for describing liquid structure. Potential profile has been changed two ways; firstly, by changing the local field correction functions proposed by Vashishta-Shingwi (VS) and Ichimaru-Utsumi (IU) and secondly, by changing the model parameter Z_s (the s electron occupancy number). We observe that the variation of Zs and local field correction functions changes the potential profile, especially, the depth and position of the principal minimum. Position of the principal minimum is responsible for estimation of effective HS diameter. Surface properties of the concerned systems have been changed a little bit with different values of effective HS diameter. Calculated results of γ suggest that first order approximation of PY solution for χ_T works better than that of second order.

Keywords: *Surface tension, Surface entropy, Hard sphere diameter, Liquid metals*

1. INTRODUCTION

Investigation of surface tension (γ) and surface entropy (S_v) of simple metals and their alloys in the condensed state has attracted scientists, technologists, and metallurgists for their multiple applications in science and technology as well as in the academic research [1-7] since a few decades. Determination of γ is an essential factor to explain several phenomena, such as gas bubble nucleation, gas absorption, and undergoing metal reactions [1]. Along with these numerous physical characteristics, some material processing methods such as sintering, soldering, dying, brazing and wetting, etc. [1-12] require knowledge of physics at surface for better understanding.

Statistical mechanical theory [11, 13-15], density functional theory [16, 17], various semi-empirical models [1] etc. had been developed over the last 70 years for the investigation of surface properties theoretically. Apart from the theoretical methods mentioned above, some experimental techniques, such as levitated drop [18, 19], sessile drop [20], drop weight [20, 21], oscillation drop [22] and others are now used for measurement of surface tension. The limitation of the experimental techniques is that they often provide a range of data rather than a single value. The reason behind this deviation is as follows. Melting point of the concerned metals is usually high and as a result, it is very difficult to remove all contaminants completely both from the environment and the surface of the specimen for measurement of the interfacial tensions.

Evans, in 1974 [11], investigated γ of several liquid simple metals using the statistical mechanical theory where for effective interionic interaction, they had chosen pseudopotential model, although the conclusions for the studied metals underestimated the experimental data that was available in contrast to the above studies. Korkmaz et al. [23] applied Fowler's formula [14] which has been derived using statistical mechanical theory. The authors in ref. [23] also applied it to liquid transition metals and the calculated results were also observed to be good in agreement with the available experimental data. However, Fowler's formula only gives us an approximated value for a potential which has a long oscillating tail of Friedel-type. If a potential contains such a long tail, the integrand of Fowler's integrand must be cut at a valid inter atomic distance to avoid divergency. In another study, Sonvane group [12] studied the atomic transport, such as viscosity and diffusion coefficients and surface properties, γ and S_v of the concerned systems by applying the formula proposed by Born and Green [24]. In their calculation they used different local field correction functions are chosen in the pseudopotential. To avoid the divergency observed in case of Friedel-type oscillating tail, recently, Amin et al. [6] extended Mayer's empirical formula [25] by utilizing second order Percus-Yevick (PY) solutions of χ_T for calculating γ of some liquid transition metals. The calculated results were also found excellent in agreement with experiments. Following the work of Amin et al., recently, Uddin et al. [26] also derived a simple but efficient formula for γ consisting of packing fraction (η). The authors in ref. [26] applied it to the liquid alkali metals and found efficient for calculating γ. It is noted that, if the vapor pressure is neglected from the expression derived by Reiss et al. [27] for γ, it reproduces the formula developed by Uddin et al. To our best knowledge, no studies using both first and second order approximations of PY solutions of χ_T have been reported yet simultaneously for the concerned systems. However, if is understood, one may simply determine S_v by taking negative derivative of γ with respect to temperature. In this regard, we would like to point out that the number density (ρ) as well as the η of liquid metals changes relatively little around melting temperatures as a result of temperature changes. Assuming this, Gosh et al. [2] derived a formula for S_v [2] and then applied to the liquid less simple metals including the concerned systems. Different, from the work of Gosh et al., current study focuses the effect potential profiles changed by the variation Z_s local field correction functions on the calculation of surface properties.

Effective pair potentials derived from the various model potentials [28, 29] have significant influences on the different physical properties of liquid metals [26, 30]. In the meantime, effective pair potential derived from both Bretonnet and Silbert's [28] pseudopotential model is observed efficient in calculating atomic transport and surface properties of liquid metals [26, 30]. The attractive feature of BS model is that it has included both sp and d band contributions of liquid transition metals. Besides this feature, it is easily handled numerically and the local form of the model permits the extension of the model for other liquid metals where the consideration of $sp-d$ hybridization is important. The concerned metals Zn, Sn, and Pb lie at the end of the transition metals of the $3d$, $4d$, and $5d$ series. Although they have completely filled d-bands, the effect of $sp-d$ hybridization is still present and strong [2]. Any specific theoretical approach has not yet been applied to explain their hybridization effect in detail. Consequently, this impact can be roughly explained by altering Z_s of $s(sp)$ and d band's s electrons. As long as the charge transfer computation with self-consistency condition permits it, there are no restrictions on using appropriate values of Z_s. But J. A. Moriarty [31] suggested that effective number of nearly free sp electrons for $3d$ and $4d$ transition metals should lie within the range like $1.1 \leq Z_s \leq 1.7$. For quantitative analysis, pseudopotential must be taken into consideration for the exchange and correlation effect. Two sophisticated local field correction functions that follow the compressibility sum rules' self-consistency are Ichimaru-Utsumi (IU) [32] and Vashishta-Shingwi (VS) [33]. In this study, we have applied both different Z_s values and local correction functions to see the role of effective pair interaction for the determination of surface properties namely γ and S_v.

Surface properties, γ and S_v depend on the structure of liquid metals [5]. From the study of Gosh et al. [5], it has been observed that the determination of effective HS diameter (σ) depends on the applied theory of structure. Effective HS diameter is the key component of the employed theories of this study. Structure of liquid metals (pair correlation function, $g(r)$), can be calculated using various methods [34], for example, perturbation theories [35-37], integral equation theory [28] and computer simulation method [38]. Previous studies claimed that HS interaction can properly explain the structure of less simple metals [2, 39]. Following the success, we have employed the mentioned theories within hard-sphere Percus-Yevick (HSPY) as the reference system in the present study without trying any other reference [40]. LWCA perturbation theory [41] have been applied in this calculation. The base of this theory is the WCA [35]. The term LWCA was first used to describe the elemental simple metallic systems, according to Kumaravadivel and Evans [42]. This theory already has been successfully applied to study the surface properties [2, 4, 5]. We should note here that the understanding of σ is necessary to explain HSPY liquid system properly. σ has been determined by using the transcendental equation of the LWCA theory.

In this paper, firstly, we have calculated γ and S_v of liquid metals Pb, Sn, and Zn by BS pseudo-potential for electron-ion interaction with LWCA perturbation theory for liquid structure. This study is a serious test to see whether the local correction function and Z_s can provide reliable results for surface tension and surface entropy or not. Organization of this study is as follows. In section 2, we have described employed LWCA theory, model potential and the expressions for surface tensions and surface entropy in brief. The calculated results are presented in section 3 and then we discuss the results with arguments. Finally we summarize the outcomes of this paper in section 4.

2 THEORY

In this section, we have described employed theories, in brief.

2.1 Bretonnet and Silbert model potential

BS introduced a model potential for liquid transition metals which can explain both the s-p and d-bands contributions within the pseudopotential formalism.

$$u(r) = \begin{cases} \sum_{m=1}^{2} B_m e^{\left(-\frac{r}{ma}\right)} & for\ r\ <\ R_c \\ -\frac{Z_s e^2}{r} & for\ r\ >\ R_c \end{cases} \tag{1}$$

where, R_c, a and Z_s, respectively, are the core radius, softness parameter and effective s-electron occupancy number. The unscreened form factor for deriving interionic interaction is as follows

$$V_0(q) = 4\pi\rho a^3 [\frac{B_1 J_1}{(1+a^2q^2)^2} + \frac{8B_2 J_2}{(1+4a^2q^2)^2}] - \frac{4\pi\rho Z_s e^2 \cos(qR_c)}{q^2}, \tag{2}$$

B_m and J_m in Eq. (2) are given in ref. [43] and ρ is the number density. Effective interionic interaction obtained from Eq. (2) is given by

$$v(r) = \frac{Z_s^2 e^2}{r}\left(1 - \frac{2}{\pi}\int F_N(q)\frac{\sin(qr)}{q}dq\right). \tag{3}$$

$F_N(q)$ in Eq. (3) is the normalized energy wave number characteristic can be expressed as,

$$F_N(q) = (\frac{q^2}{4\pi\rho Z_s e^2})^2 w_0^2(q)[1 - \frac{1}{\epsilon(q)}][1 - G(q)]^{-1}. \tag{4}$$

$\epsilon(q)$ in Eq. (4) is the dielectric screening function, This dielectric screening function depends on the local field correction function, $G(q)$ and can be written as

$$\varepsilon(q) = 1 - \left[\frac{\frac{4\pi e^2}{q^2}\chi(q)}{1+\frac{4\pi e^2}{q^2}G(q)\chi(q)}\right]. \tag{5}$$

$\chi(q)$ in Eq. (5) is the Lindhard function. The local field correction function proposed by Ichimaru and Utsumi (IU) [32] is given by

$$G(q) = \frac{a_0 Q^2}{Q^2 + a_1}, \tag{6}$$

where a_0 and a_1 are coefficients calculated by IU in [32].

From Eq. (3) it is evident that Z_s and $G(q)$ are able to change the effective interionic interaction. Therefore, to see the role of potential, here, we have chosen another well-known $G(q)$ proposed by Vashishta and Singwi [33] which has the following form

$$G(q) = A(1 - e^{-BQ^2}), \tag{7}$$

where A and B are parameters calculated by VS and depend on the number density, ρ and effective valance, Z_s. Q in Eq (6) and Eq (7) denotes the ratio q/q_F. Here q_F is Fermi wave vector.

2.2 LWCA Perturbation theory

Meyer et al. [40] proposed LWCA perturbation theory for calculation of $g(r)$ of metals in the condense state. It has been developed based on the WCA theory [35]. In the WCA theory, the blip function is expressed as

$$B(r) = Y_\sigma(r)[e^{(-\beta v(r))} - e^{(-\beta V(r))}] \tag{8}$$

where $v(r)$ and $V(r)$ are respectively the soft and the hard part of the effective pair potentials. The inverse of temperature times Boltzmann constant is denoted by β. The cavity function, $Y_\sigma(r)$ in Eqn. (8), is continuous at $r = \sigma$ and connected to the HS distribution function. It is also identical to the hard sphere distribution function, $g_\sigma(r)$, for $r > \sigma$. We adhere to Meyer et al. [41] when evaluating $y(r)$. In LWCA, plotting of the function $r^2 b(r)$ with respect to r provides in two pointed teeth which are approximated using right triangle. After taking Fourier transformation, the blip function, $B(r)$, in q space is written as

$$B(q) = 4\pi \int_0^{\infty} B(r) \frac{\sin{(qr)}}{qr} dr \tag{9}$$

Expanding the integral according to Bessel's function, and then taking the thermodynamic constraint $B(q = 0) = 0$ we get a transcedental equation which is as follows.

$$\beta v(\sigma) = ln \frac{-2\beta\sigma v'(\sigma)+Y+2}{-\beta\sigma v'(\sigma)+Y+2} = \varphi(r), \tag{10}$$

where $v'(r)$ is the first derivative of v with respect to r. After plotting of the right and left side of the Eq. (10), we have estimated effective HS diameter, $\sigma,$ from the r position of the intersecting curves. It can also be solved by numerically. Packing fraction η is conected to the HS diameter by the relation $\eta = \frac{1}{6}\pi\rho\sigma^3$.

2.3 *Surface Entropy*

Fowler's formula [14] based on statistical mechanical theory is given below

$$\gamma = \frac{\pi\rho^2}{8} \int_0^{\infty} \frac{dv}{dr} g(r) r^4 dr \tag{11}$$

where $g(r),\ \rho$ and σ respectively denote pair distribution function, ionic number density and interionic interaction. The value of η depends on metal to metal as well as temperature. Considering these assumptions and applying the HS interaction, Gosh et al. [2] derived a surface entropy formula which is as follows.

$$S_V = \frac{\pi\rho^2 k_B \sigma^4 (2-\eta)}{16(1-\eta)^3}\left[1 - 0.252\frac{\sigma_m}{\sigma}\left(\frac{T}{T_m}\right)^{1/2}\right] - \frac{0.189\pi\rho^2 k_B \sigma^3 \eta(5-2\eta)}{16(1-\eta)^4}\left(\frac{T}{T_m}\right)^{1/2}. \tag{12}$$

In this work, we have used Eq. (12) for calculation of surface entropy.

2.4 *Surface Tension*

Liquid metals are usually dense. Therefore, they need complex theories to describe them properly. The repulsive inter-molecular interaction is usually responsible for determination of structure of liquid metals, and based on this assumption, numerous ideas have been already proposed [35, 45-47]. From this concept, we can infer that the intermolecular correlations are governed by the shape of the molecules. A hard sphere's potential is often entirely repulsive. Due to this, only the repulsive portion of the hard sphere potential should be mimicked when simulating the interaction of real liquid systems [48, 49].

This presumption led to the development of many equations that were successfully used to calculate atomic transport [49] and surface properties [1, 6]. Mayer [25] suggested the empirical link given below for the variables surface tension, γ and compressibility, χ, which is based on the HS interaction is expressed by the following equation,

$$\chi\gamma = \sigma\left[\frac{(2-3\eta+\eta^3)}{4(1+2\eta)^2}\right]. \tag{13}$$

Amin et al. [6] developed a surface tension formula using effective σ based on this empirical relationship for liquid noble and transition metals. They did this by employing an expression for isothermal compressibility (χ_T) derived from the PY solution's second order approximation [50]. The expression of Amin et al, for surface tension is as follows

$$\gamma = \frac{\sigma\rho k_B T[2\eta(4-\eta)+(1-\eta)^4](2-3\eta+\eta^3)}{4(1+2\eta)^2(1-\eta)^4}, \tag{14}$$

where T, and k_B respectively denote the temperature, and Boltzmann constant. An alternative method of the integral equation method, which is rational function approximation has been used. The compressibility equation that results from the PY solution's first order approximation can be expressed as,

$$\chi = \frac{(1-\eta)^4}{\rho k_B T(1+2\eta)^2} \tag{15}$$

If we substitute Eq. (15) into Eq. (13), γ, can be expressed as

$$\gamma = \frac{\sigma\rho k_B T(2+\eta)}{4(1-\eta)^2}. \tag{16}$$

Eq. (16) and Eq. (14) have been used for calculating γ of the concerned metals in this work.

3 RESULTS AND DISCUSSION

The calculated results of γ and S_v of the concerned systems have been presented at first and then we discuss the presented results for various Z_s values and local field correction functions with arguments. The second and first order approximations presented in Eq. (14) and Eq. (16), respectively, is used to calculate γ. In order to calculate S_v, we have used Eq. (12). Temperature-dependent η and the associated σ is the main component of all the expressions mentioned. By combining the BS pseudopotential with LWCA perturbation theory, we have determined them. Potential profiles, obtained by tuning the model parameter Z_s and by utlizing the local field correction functions, are the most important components of this computation.

For deriving the effective interionic interaction from BS pseudo-potential requires three parameters R_c, a and Z_s which are required to fix at first. Among them R_c and a are chosen from the ref. [2]. In this study, different fractional values of R_c and a are chosen to see the $sp-d$ hybridization effect in the calculation. All input parameters required for this calculation are listed in Table 1. Besides this, the choice of local field correction function also has a big impact on the calculation of $v(r)$. As a result, we have included two separate local field correction functions proposed by IU [32] and VS [33] as well. Utilizing the all parameters mentioned the potential profile obtained from them , $v(r)$ is shown in Fig. 1.

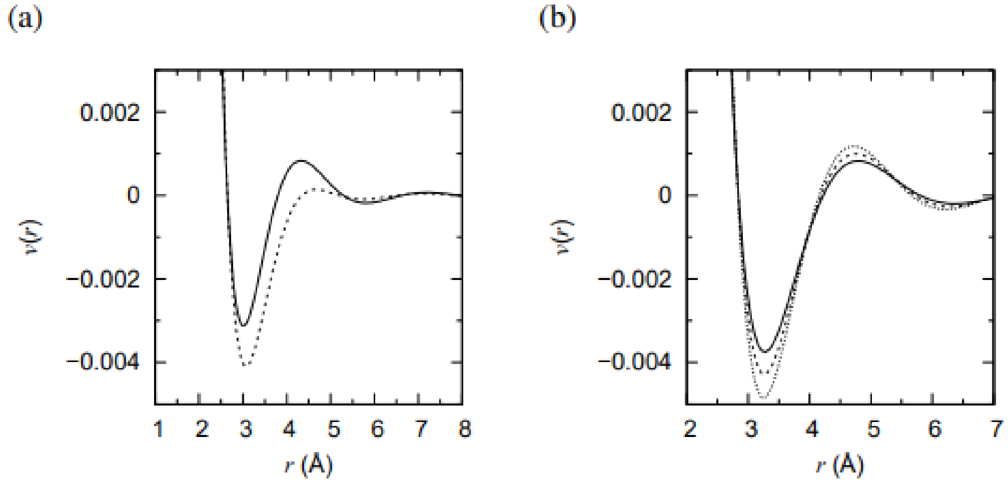

Fig. 1: Represents the variation of effective pair potential, $v(r)$ with inerionic distance r. In (a) solid and dash line represent $v(r)$ of representative liquid Sn derived employing the IU and VS local field correction functions, respectively whereas in (b) solid, dash and dot line represent $v(r)$ of representative liquid Pb derived using effective valence Z_s as 1.5, 1.6 and 1.7, respectively.

Table 1: Values of the input parameters used in this study

Metals	T(K)	T_m(K)	ρ(Å $^{-3}$)	ρ_m (Å $^{-3}$)	R_c $(a.u.)$	a $(a.u.)$
Pb	613	600	0.0310	0.0310	1.47	0.307
Sn	523	505	0.0353	0.0355	1.30	0.273
Zn	723	692	0.0602	0.0605	1.27	0.285

Potential profile has been resulted from the sensitive balance between the attractive and repulsive pair interactions of atoms in concerned metals. The reason behind these interactions occurring in the pseudopotential formalism is due to direct interaction between various ion cores and indirect interaction araised from conduction electrons. Local field correction functions in the dielectric function play significant roles in the above cases. When VS is used instead of IU, we observe from Fig. 1(a) that the potential well depth increases significantly and the first minimum's position shifted towards right a little bit. From Fig. 1(b), we observe that the depth of the potential well increases with the increasing values of Z_s by keeping the position of first minimum fixed.

As we said earlier that σ, and η are the primary ingredients of the employed theories. We have applied the liquid structure LWCA theory in conjunction with the derived effective interionic interaction, $v(r)$ to calculate them. Intersecting curves of the transcendental equation [Eq.(10)] provides σ which is shown in Fig. 2(a). Then, using the equation $\eta = \frac{1}{6}\pi\rho\sigma^3$ [39, 49], η is calculated. In Table 2 and Table 3, along with other relevant experimental and theoretical data, the calculated values of S_v and γ are presented, respectively. Since the estimation of σ relies on the liquid structure, it is crucial to present $g(r)$ for a few example systems. As a representative, the calculated $g(r)$ using LWCA theory for liquid Pb is presented in Fig. 2(b) with experimental data

[51]. We observe from Fig. 2(b) that the calculated $g(r)$ values are consistent with the corresponding experimental data.

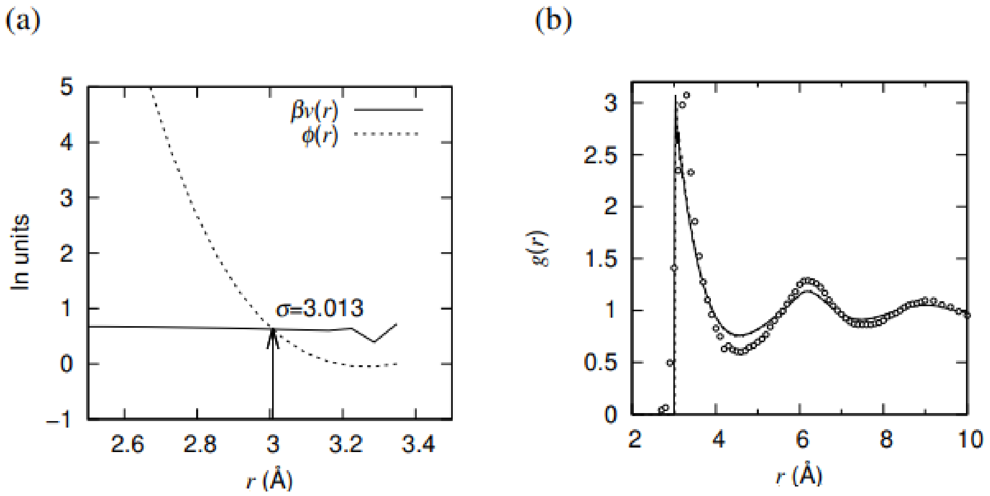

Fig. 2: (a) shows the graphical method for calculation of effective HS diameter. (b) shows the calculated $g(r)$ using IU and VS local field correction functions, presented by solid and dash curves, respectively, for liquid Pb with a fixed Z_s value of 1.6, are compared with experimental data [51] presented by symbol circles.

Table 2: Calculated data of Surface Entropy (S_V) in (Nm^{-1}Kg $^{-1}$ × 10^{-3}) are presented with the available theoretical values [2] and experimental data [13]

Metals	Z_s	σ(Å)		σ_m(Å)		η		S_V		Theo.		Exp.
		IU	VS	IU	VS	IU	VS	IU	VS	[2]	[13]	[13]
Pb	1.5	3.008	3.050	3.015	3.054	0.442	0.461	0.066	0.069	0.067	0.16	0.13
	1.6	3.013	3.020	3.016	3.060	0.444	0.447	0.063	0.065			
	1.7	3.022	3.010	3.023	3.057	0.448	0.443	0.067	0.064			
Sn	1.6	2.786	2.837	2.790	2.843	0.400	0.442	0.061	0.067	0.062	0.19	0.07
	1.7	2.797	2.834	2.801	2.842	0.404	0.421	0.062	0.066			
	1.8	2.784	2.843	2.790	2.845	0.399	0.426	0.061	0.068			
Zn	1.3	2.462	2.529	2.470	2.533	0.470	0.509	0.106	0.109	0.107	0.20	0.17
	1.4	2.476	2.537	2.480	2.541	0.479	0.515	0.107	0.102			
	1.5	2.487	2.545	2.489	2.548	0.485	0.519	0.107	0.100			

Table 2 shows that estimated σ value increases when Z_s value is considered larger in the potential. It is also seen that VS field with Z_s value provides a little bit larger value of σ than that of IU. It is due to the fact that the position of first minimum of VS which is observed at a little bit larger r than that of IU. We also observe that the effective σ values at the calculated temperature (above melting point) is slightly lower than those obtained at the melting temperature, σ_m. The reason behind this is as follows. When two liquid atoms move closer as a result of the increased kinetic energy due to increased temperature, the average distance of closest atoms decreases [49]. This behavior is also found consistent with our previous study [2]. These outcomes further demonstrate the precision and constancy of our calculations.

Next, using the obtained σ values S_v of the concerned systems are calculated by applying the Eq. (12). We have listed calculated values inTable 2. The available theoretical values [2, 13] and experimental data [13] are also presented in Table 2. It is seen from Table 2 that obtained values using VS are found a little bit larger than those of IU. The calculated results, using both IU and VS, are found smaller in magnitudes from experimental data [13] except liquid Sn. For liquid Sn, observed surface entropy is well-matched with the experimental data. With increasing Z_s values, the variation of S_V values using IU and VS is negligible and VS follows decreasing trend.

Table 3: Calculated data of Surface Tension (γ) in (Nm^{-1}) with the available experimental data [20, 19]. Calc.1 and Calc.2 represent the results obtained using first and second order approximations of PY solutions of isothermal compressibility, respectively.

Metals	Z_s	γ				
		Calc.1		Calc.2		Expt. [20, 19]
		IU	VS	IU	VS	
Pb	1.5	0.217	0.257	0.141	0.153	0.441
	1.6	0.221	0.227	0.143	0.144	
	1.7	0.229	0.218	0.145	0.142	
Sn	1.6	0.138	0.169	0.109	0.120	0.551
	1.7	0.144	0.172	0.112	0.122	
	1.8	0.137	0.175	0.109	0.123	
Zn	1.3	0.516	0.745	0.294	0.352	0.767
	1.4	0.556	0.780	0.305	0.360	
	1.5	0.590	0.831	0.314	0.371	

Similarly findings of γ of the concerned systems are presented in Table 3. From Table 3 we have seen that obtained γ values using VS are found larger than those of IU. The calculated results, using both IU and VS, are found smaller in magnitudes from experimental data [13] except for liquid Zn. For liquid Zn, observed value of γ is well-matched with the experimental one [19, 20]. For both IU and VS local field, first order PY approximation of χ_T works better than the that of second order approximation. With increasing Z_s values, the variation of γ values using both IU and VS is significant but found random.

4 CONCLUSIONS

In the present study we have investigated γ and S_v of liquids Pb, Sn, and Zn near melting points using the HS theories of liquid metals. For investigation, we have used well-known BS pseudopotential model with IU and VS local filed correction functions in conjunction with LWCA perturbation theory. We have also applied fractional values of Z_s to see the hybridization effect on the calculation of surface properties. Considering the presented results and discussion, following conclusions are drawn:

(i) BS pseudopotential in conjunction with LWCA theory can be applied for the study of γ and S_v of liquids Pb, Sn and Zn.

(ii) The effective HS diameter increases with the increased values of Z_s.

(iii) The calculated results of $S_v$using IU local field correction functions are slightly smaller than those obtained using VS with compared to the available literature values. The variation of Z_s has the little influence on calculation of surface entropy.

(iv) Calculated results of γ for the concerned systems are found close to the available experimental data when it is dealt with first order approximation. Hybridization effect is also essential for liquid Zn.

REFERENCES

[1] T. Iida and R. IL Guthrie, The Thermophysical Properties of Metallic Liquids, Volume 1: Fundamentals. Oxford University Press, 2015.

[2] R. C. Gosh, A. Z. Ziauddin Ahmed and G. M. Bhuiyan, Investigation of surface entropy for liquid less simple metals, The European Physical Journal B **56** (2007) 177-181.

[3] B. Jürgen, D. Chatain and I. Egry, Surface tension of liquid binary alloys–theory versus experiment, International Journal of Materials Research **100** (2009) 53-58.

[4] S. Korkmaz and S. D. Korkmaz, A comparative study of electrical resistivity of liquid alkali metals, Computational materials science **37** (2006) 618-623.

[5] R. C.Gosh,M.R.Amin,A. Z. Ziauddin Ahmed, I. M. Syed and G.M. Bhuiyan, Calculation of surface entropy of liquid transition and noble metals, Applied surface science **258** (2012) 5527-5532.

[6] M. R. Amin, R. C. Gosh and G. M. Bhuiyan, Surface tension of liquid transition and noble metals, Journal of non-crystalline solids **380** (2013) 42-47.

[7] R. C. Gosh, R. Das, S. C. Sen and G.M. Bhuiyan, Surface entropy of liquid transition and noble metals, Surface Science **637** (2015) 63-68.

[8] R. C.Gosh, M. R. Amin and G. M. Bhuiyan, Atomic transport for liquid noble and transition metals using scaling laws, Journal of Molecular Liquids **188** (2013) 148-154.

[9] S. D. Korkmaz and S. Korkmaz. Determination of surface properties of liquid simple metals, Optoelectronics and Advanced Materials-Rapid Communications **3** (2009) 116-119.

[10] S. D. Korkmaz and Ș. Korkmaz, Investigation of atomic transport and surface properties of liquid transition metals using scaling laws, Journal of Molecular Liquids **150** (2009) 81-85.

[11] R. Evans, A pseudo-atom theory for the surface tension of liquid metals, Journal of Physics C: Solid State Physics **7** (1974) 2808-2830.

[12] Y. A. Sonvane, P. B. Thakor and A. R. Jani, Atomic transport and surface properties of some simple liquid metal using one component plasma system, Journal of Theoretical and Applied Physics **6** (2012) 1-6.

[13] T. Itami and M. Shimoji, The hard-sphere model for the surface entropy of liquid metals, Journal of Physics F: Metal Physics **9** (1979) L15.

[14] R. H. Fowler, A tentative statistical theory of Macleod's equation for surface tension, and the parachor, Proceedings of the Royal Society of London. Series A-Mathematical and Physical Sciences **159** (1937) 229-246.

[15] J. G. Kirkwood and F. P. Buff, The statistical mechanical theory of surface tension, The Journal of Chemical Physics **17** (1949) 338-343.

[16] Y. Martinez-Raton, E. Velasco, A. M. Somoza, L. Mederos and T. J. Sluckin, Theoretical study of the anomalous surface tension properties of liquid crystals, The Journal of chemical physics **108** (1998) 2583-2593.

[17] N. D. Lang and W. Kohn, Theory of metal surfaces: charge density and surface energy, Physical Review B **1** (1970) 4555-4568.

[18] I. Egry, G. Lohoefer and G. Jacobs, Surface tension of liquid metals: results from measurements on ground and in space, Physical review letters **75** (1995) 4043-4046.

[19] K. Nogi, K. Ogino, A. McLean and W. A. Miller, The temperature coefficient of the surface tension of pure liquid metals, Metallurgical Transactions B **17** (1986) 163-170.

[20] B. J. Keene, Review of data for the surface tension of pure metals, International Materials Reviews **38** (1993) 157-192.

[21] A. W. Peterson, H. Kedesdy, P. Keck and E. Schwarz, Surface tension of undercooled liquid cobalt, J. App. Phys. **29** (2009) 213-216.

[22] W. J. Yao, X. J. Han, M. Chen, B. Wei and Z. Y. Guo, Surface tension of undercooled liquid cobalt, Journal of Physics: Condensed Matter **14** (2002) 7479-7485.

[23] S. D. Korkmaz and Ş. Korkmaz, Investigation of surface properties of liquid transition metals: surface tension and surface entropy, Applied surface science **257** (2010) 261-265.

[24] M. Born and H. S. Green, A general kinetic theory of liquids III. Dynamical properties, Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences **190** (1947) 455-474.

[25] S. W. Mayer, A molecular parameter relationship between surface tension and liquid compressibility, The Journal of Physical Chemistry **67** (1963) 2160-2164

[26] M.S. Uddin, R.C. Gosh, G.M. Bhuiyan, Investigation of surface tension, viscosity and diffusion coefficients for liquid simple metals, Journal of Non-Crystalline Solids **499** (2018) 426-433, https://doi.org/10.1016/j.jnoncrysol.2018.07.014.

[27] H. Reiss, J. L. Lebowitz, Aspects of the statistical thermodynamics of real fluids, The Journal of Chemical Physics **32** (1960) 119-124.

[28] J.L. Bretonnet and M. Silbert, Interionic interactions in transition metals. application to vanadium, Phys. Chem. Liq. **24** (1992) 169-176. https://doi.org/10.1080/00319109208027266.

[29] M.W. Finnis, J.E. Sinclair, A Simple Empirical N-Body Potential for Transition Metals, Philos. Mag. A **50** (1984) 45-55. https://doi.org/10.1080/01418618408244210.

[30] R.C. Karmkar, R.C. Gosh, Validity of the Stokes-Einstein relation in liquid 3d transition metals for a wide range of temperatures, J. Mol. Liq. **328** (2021) 115434. https://doi.org/10.1016/j.molliq.2021.115434.

[31] J. A. Moriarty, Analytic representation of multi-ion interatomic potentials in transition metals, Phys. Rev. B **42** (1990) 1609-28.

[32] Ichimaru and K. Utsumi, Analytic expression for the dielectric screening function of strongly coupled electron liquids at metallic and lower densities, Physical Review B **24** (1981) 7385-7388; https://doi.org/10.1103/physrevb.24.7385.

[33] P. Vashishta and K.S. Singwi, Electron Correlations at Metallic Densities. V., Physical Review B, 6 (1972) 875-887; https://doi.org/10.1103/physrevb.6.875.

[34] J.P. Hansen and J. R. McDonald, Theory of Simple Liquids, Academic Press, (1976).

[35] J.D. Weeks, D. Chandler and H. C. Andersen, Role of Repulsive Forces in Determining the Equilibrium Structure of Simple Liquids, The Journal of Chemical Physics **54** (1971) 5237-5247, https://doi.org/10.1063/1.1674820.

[36] A. Ishihara, The Gibbs-Bogoliubov inequality, J. Phys. A **1** (1968) 539.

[37] J. A. Barker and D. Henderson, Perturbation Theory and Equation of State for Fluids. II. A Successful Theory of Liquids, The Journal of Chemical Physics 47 (1967); https://doi.org/10.1063/1.170168.

[38] R. L. McGreevy, Understanding liquid structures, Journal of Physics: Condensed Matter, 3 (1991) F9-F22; https://doi.org/10.1088/0953-8984/3/42/002.

[39] M. Shimoji, Liquid Metals: An Introduction to the Physics and Chemistry of Metals in the Liquid States Academic, London (1977) pp: 104-105.

[40] M. Ross, H. E. DeWitt, and W. B. Hubbard, Monte Carlo and perturbation-theory calculations for liquid metals, Phys. Rev. A **24** (1981) 1016-1020; https://doi.org/10.1103/PhysRevA.24.1016.

[41] A. Mayer, M. Silbert and W.H. Young, Chem. Phys. **49** (1980) 147-152.

[42] R. Kumaravadivel and R. Evans, The entropies and structure factors of liquid simple metals, Journal of Physics C: Solid State Physics **9** (1976) 3877-3903; https//doi.org/10.1088/0022-3719/9/21/008.

[43] J. L. Bretonnet and M. Silbert, Interionic interactions in transition metals. Application to vanadium, Physics and Chemistry of Liquids **24** (1992) 169-176.

[44] N. F. Carnahan and K. E. Starling, Equation of state for nonattracting rigid spheres, The Journal of chemical physics **51** (1969) 635-636.

[45] H. C. Andersen, T. Chern. Phys. 56, 3812 (1972); D. Chandler and. TD Weeks, Phys. Rev. Lett **25** (1970) 149.

[46] H. C. Andersen, and David Chandler. "Optimized Cluster Expansions for Classical Fluids. I. General Theory and Variational Formulation of the Mean Spherical Model and Hard Sphere Percus-Yevick Equations." The Journal of Chemical Physics **57** (1972) 1918-1929.

[47] H. C. Andersen, John D. Weeks, and David Chandler. "Relationship between the hard-sphere fluid and fluids with realistic repulsive forces." Physical Review A **4** (1971) 1597.

[48] H. Reiss, Scaled particle methods in the statistical thermodynamics of fluids, Advances in Chemical Physics (1965) 1-84

[49] P. Protopapas, H. C. Andersen and N. A. D. Parlee, Theory of transport in liquid metals. I. Calculation of self-diffusion coefficients, The Journal of Chemical Physics **59** (1973) 15-25.

[50] M. Shimoji and T. Itami, Atomic transport in liquid metals. Aedermannsdorf: Trans Tech Publications, 1986.

[51] Y.Waseda, The Structure of Non-crystalline Materials, McGraw Hill, Newyork, 1980.