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Investigation of Physicochemical Property and Transport Coefficients of Liquid Aluminum (Al): Temperature Dependence Revisited

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Abstract

The physicochemical property (PHP) and transport coefficients (TC) of liquid aluminum (Al) have been studied based on how they change with temperature (T), using the microscopic first-order perturbation hard sphere (HS) theory of liquid metals. PHP involves surface tension (S_T) and isothermal compressibility (χ_T) of the surface properties. On the other hand, TC properties such as shear viscosity (η) and diffusion (D) are investigated for the same footing. The effective hard-sphere diameter (σ), along with packing fraction (Ω), and the effective pair potential ($V_{ij}(r)$) are the basic ingredients of the first-order perturbation microscopic theory in the present inquisition. To facilitate accurate computational analysis, these constituents are assessed utilizing a local pseudopotential and the linearized Weeks-Chandler-Andersen thermodynamic perturbation theory (LWCA). The calculated results, when juxtaposed with the existing experimental data and estimated theoretical values, indicate that the LWCA predicts a slight temperature-dependent divergence in the study of Al. The root cause of this deviation in the uncertainty level of the results for Al is examined, and possible reasons are explained.

Keywords

Surface Tension (S_T), Isothermal Compressibility (χ_T), Shear Viscosity (η), Diffusion (D), Bretonnet-Silbert Pseudopotential, LWCA Theory

1. Introduction

Because of numerous uses of PHP (S_T, χ_T) and TC (η, D) in both industry and academia, S_T [1]-[6], χ_T [7]-[14], η [12], and D [13] have drawn the attention of scientists, technologists, and metallurgists, respectively. S_T markedly affects numerous processes, including the nucleation of gas bubbles, gas absorption, the creation of non-metallic inclusions, and metal reactions [1]-[6]. Legionary physical features associated with χ_T into material processing procedures, such as soldering, brazing, sintering, dyeing, and wetting, necessitate an understanding of surface physics for enhanced insight. Moreover, η and D can also have a significant effect in the process of binary solidification and in the regulation of the rate at which biological and new functionality of material growth procedures occur [12] [13]. This suggests that structural and thermodynamic factors might significantly influence surface tension and, consequently, the atomic transport properties of liquid metals. For instance, shear viscosity and diffusion coefficients are two examples of features that can be affected by these processes. Consequently, examining the potential interconnection among the aforementioned traits presents a compelling challenge. Here, a theory that best explains the liquid structure and thermodynamics of the systems being studied is required.

The purpose of investigations of PHP and TC for different thermodynamic states $T = 950$, 1050, and 1150 K, respectively, is fourfold. First, even though Al is one of the most often utilized metals, little is known about the inherent usefulness of its S_T. Keene [1] investigation demonstrated that S_T of Al at temperatures close to its melting point (943K) is between 850 - 1100 mN/m. This S_T has been measured by different researchers using different methods. The source of this significant dispersion, markedly above the usual error of S_T surface tension measurements (2% - 3%), is unequivocally the heightened sensitivity of the surface characteristics of molten aluminum to oxygen. In the literature review [1]-[6], two distinct groupings of S_T values can be recognized. S_T values ranging from 850 to 900 mN/m were found from meticulous tests conducted by multiple teams under diverse atmospheric conditions either the sessile drop technique or the maximum bubble pressure (MBP) approach. The temperature coefficient of S_T ($\mathrm{d}S_T/\mathrm{d}T$) in these studies was found to range from -0.10 to -0.20 mN m^{-1} K^{-1} [1]. Comparable values have recently been acquired via the contactless oscillating droplet tech0nique [2], and those were between 1030 and 1100 mN/m. Goumiri and Joud [3] were the first to quantify a high S_T value (1050 mN/m) with a sophisticated sessile drop experiment conducted within an Auger spectroscopy chamber following in situ cleaning of the aluminum surface. These authors assert that experimental results S_T about 850 mN/m pertain to aluminum surfaces coated with a monolayer of adsorbed oxygen. Subsequently, a significant value of approximately 1090 mN/m was observed in MBP tests [4] [5]. Recently, Sarou-Kanian *et al.* [6] determined $S_T^{mp} = 1024$ (±48) mN/m by extrapolating to the melting point of Al using a contactless approach at temperatures ranging from 1500˚C to 1900˚C in various neutral or reducing atmospheres. These analyses all indicated a conclusive point that the limitation of experimental facts. Second, only a small number of theoretical studies have been undertaken to examine S_T, χ_T, η, and D sequentially, utilizing the same ingredients from empirical or semi-empirical models [7]-[14] for liquid Al, with only a handful achieving success. Furthermore, to our knowledge, liquid Al has not been investigated for its thermodynamic states at temperatures of 950, 1050, and 1150 K, utilizing the same parameters from the initial conditions to the end results in accordance with any microscopic theory for S_T, χ_T, η, and D, respectively. Third, the dynamic features of interest for theoretical investigation have already been evaluated by many experimentalists [1]-[6]. Fourth, experimental results for static structure factors for elemental liquid Al are not available in the literature at the thermodynamic state in question [4]. Therefore, the structural requirements are crucial for making accurate assumptions about liquid Al at those temperatures.

At the same time, the literature review says that many studies have looked into the statistical mechanical theory and the S_T of certain simple liquid metals, and these reviews have pointed out significant shortcomings. First, a specific study utilizes the approximate value [8]. This value induces divergence if the potential possesses an extensive Friedel-type oscillatory tail. Avoiding this divergence is crucial for achieving the appropriate ST. It is necessary to truncate the integrand at a specific interionic distance to prevent the divergence of the Friedel-type oscillatory tail. Second, the measurement and calculation of S_{T} using transport coefficients provide significant challenges from both experimental and theoretical viewpoints [9]-[14]. Mayer's empirical method [7] was utilized to assess the temperature variation and S_T of liquid Al. A first-order approximation of Percus-Yevick [15]-[21] was then employed for the estimation of χ_T. Sutherland's [22], latterly development technique was applied for the estimation of the η, and D. σ and Ω were the key ingredients of this estimation. The electronic theory of metals employed in this work is based on a local pseudopotential proposed by Bretonnet and Silbert (BS) [21]. The band structure energy calculated from the pseudopotential theory provides the interionic interaction, which in turn is used to calculate static structure factors as well as other physical properties investigated here. It is worth noting that the BS pseudopotential has three parameters (core radius, R_c, softness parameters, a, and valency, Z) to be fixed to perform effective calculations. Here, values of R_c a, and Z are taken from other published work [18]. Once this is done, the rest of the calculation is completely parameter free. Moreover, the BS pseudopotential model has demonstrated efficacy in characterizing the structural [16], thermodynamics [17]-[19], and transport features [20] [21] of less simple liquid metals and their alloys. Another important ingredient of the present microscopic approach is the partial correlation function, $g_{ij}(r)$, which describes the liquid structure of the constituent ions in the liquid state. In order to determine this function, we have employed the thermodynamic perturbation theory [23] as simplified further by Meyer *et al.* [7]. The latter theory is known in literature as the Linearized Weeks-

Chandler-Andersen (LWCA) theory [24]-[26].

This paper follows a structured format. Section 2 provides a concise discussion that describes briefly relevant theories that are used in the calculations. The results of the calculation are presented and discussed in Section 3. We conclude this article with some remarks in Section 4.

2. Theory

2.1. Effective Partial Pair Potential

The local pseudopotential for the i-th component of a metallic alloy may be modeled as a superposition of two terms, [21] one inside and another outside the core,

$$Y_i(r)=\begin{cases}\sum_{m=1}^{2} B_m^i \exp\left(-\frac{r}{ma_i}\right) & \text{if } r<R_{ci}\\ -\frac{Z_i}{r} & \text{if } r>R_{ci}\end{cases} \qquad (1)$$

where a, R_{ci} and Z denote the softness parameter, core radius and the effecttive s-electron occupancy number, respectively. The term outside the core is just the bare Coulomb interaction (in atomic units) between a conduction electron and an ion. The contribution inside the core is contributed by the first two terms of the Dirichlet series arising from the inverse scattering approach. For details, see Ref [18]. The coefficients of expansion in the core depends on the parameters a_i, R_{ci}, and Z_i. Finally, the partial interionic interaction between i-th and j-th ions is

$$V_{ij}(r)=\frac{Z_iZ_j}{r}\left[1-\frac{2}{\pi}\int \mathrm{d}q F_{ij}^N \frac{\sin(qr)}{q}\right] \qquad (2)$$

where the normalized energy wave number characteristics $W_i(q)$, in Equation (3), denotes the unscreened

$$F_{ij}^N=\left[\frac{q^2}{\pi a\rho\sqrt{(Z_iZ_j)}}\right]^2 W_i(q)W_j(q)\left[1-\frac{1}{\varepsilon(q)}\right]\left[\frac{1}{1-G(q)}\right] \qquad (3)$$

form factor of the i-th com ponent obtained from the Fourier transform of $W_i(r)$ (see Equation (9)), $\varepsilon(q)$ and $G(q)$ are dielectric function and the local field factor in momentum space, respectively, with q as the amount of momentum transferred. These functions are taken from Ichimaru and Utsumi [27] because their theory satisfies both the compressibility sum rule and the short-range correlation condition.

2.2. LWCA Theory

The LWCA technique [24]-[26] was utilized in this work to calculate HSD Because it is an easily understood and theoretically accessible theory. It is well known that the first principles perturbation theory requires such a reference system which can closely resemble the concerned real system [28]. There are many experimental as well as theoretical evidence that the HS theory of liquid can describe the structure of simple and transition metals [29] [30] and their binary alloys [15]-[19]. Being prompted by the above history of success we employ HS reference system for liquid Al within the LWCA thermodynamic perturbation theory proposed by Meyer *et al.* [7] was derived from the WCA theory [25]. The Blip function in the theory stands as,

$$B(r)=Y_\sigma(r)\left[\exp\left[-\beta v(r)\right]-\exp\left[\beta v_\sigma(r)\right]\right]. \tag{4}$$

Here $v(r)$, and $v_\sigma(r)$ Here, $v(r)$ and $v(r)$ denote soft and hard sphere, HS potentials, respectively. β is the inverse temperature divided by the Boltzmann constant and $Y_\sigma(r)$ is the hard sphere cavity function and it is continuous at $r = \sigma$; σ being the effective HSD. In the linearized version of the WCA, σ is obtained from the solution of the transcendental equation [31]. Our previous work [18] mentions the solution to this equation.

2.3. Pair Distribution Function

In order to have numerical values for partial correlation function, we first calculating the Ashcroft-Langreth (AL) partial static structure factors, [32] $S_{ij}(q)$, and then take a Fourier trans- form of it,

$$g_{ij}(r)=1-+\frac{1}{(2\pi)^3\rho\sqrt{x(1-x)}}\int_0^\infty\left(S_{ij}(q)-\delta_{ij}\right)\mathrm{e}^{iq\cdot r}\mathrm{d}^3q\,, \tag{5}$$

where ρ is the ionic density of alloys. We note that calculation of $S_{ij}(q)$ requires the knowledge of the effective hard sphere diameters, σ_{ij}, which is obtained by using the linearized WCA thermodynamic perturbation theory [33].

2.4. Surface Tension (S_T), Isothermal Compressibility (χ_T), Shear Viscosity (η) and Diffusion (D)

Liquid metals have a higher density than other common liquids. As a result, clarifying liquid metals requires sophisticated concepts. The idea of repulsive intermolecular forces determines the structure of liquid metals has given rise to various ideas [34]-[37]. Molecular configuration governs intermolecular interactions. A hard-sphere potential is typically, entirely repulsive. Therefore, when modeling the interactions in real liquid systems using a rigid sphere potential, one should only reproduce the repulsive part of the potential [34]. As an alternative to the integral equation approach, a rational function approximation can be used to express the S_T equation obtained from the first-order approximation of the Percus-Yevick solution as follows:

$$\gamma=\frac{\delta\eta k_BT(2+\Omega)}{4(1-\Omega)^2} \tag{6}$$

This study employs Equations (6) to compute the S_T of the relevant system. In order to estimate the isothermal compressibility (χ_T), the first-order approximation of the Carnahan and Stirling [38] solution has been used, taking into account the rational function approximation. This approximation can also be adjusted as an alternative to the integral equation method for hard sphere fluid. The mathematical equation is presented below:

$$\chi_T = \frac{(1-\Omega)^4}{\rho k_B T\left\{2\Omega(4-\Omega)+(1-\Omega)^4\right\}} \tag{7}$$

where ρ is the ionic number density, k_B is the Boltzmann constant and T is the temperature. Furthermore, equations (8) and (9) have been utilized to get the transport coefficients η and D. Equation (8) has been examined within the context of the assumptions stated by Born and Green [14]. Conversely, equation (9) was also formulated by Sutherland [22] *et al.* from the original Stokes-Einstein equation utilizing hydrodynamic theory, as detailed in the following two equations:

$$\eta = \frac{16m^{\frac{1}{2}}}{15(k_B T)^{\frac{1}{2}}} S_T, \tag{8}$$

and,

$$D = \frac{15k_B T}{32\pi\sigma S_T m}\frac{(k_B T)^{1/2}}{m^{1/2}}. \tag{9}$$

where, m is the atomic mass of the liquid atoms.

3. Results and Discussion

In this section, we have presented the results of calculations for the S_T, χ_T, η, and D of the simple liquid Al metal at temperatures of 950 K, 1050 K, and 1150 K, respectively. The reason for choosing this liquid system due to its generally accepted lack of *sd* hybridization effects [37]. Besides, Al is a heavy polyvalent metal, and are sometimes difficult to handle theoretically, in the framework of empirical or semi empirical models. So, we have employed the microscopic self-consistent theory within the conjunction of pseudopotential as BS model potential to describe the interionic interaction of the Al simple metal for revealing the liquid state features with temperature variation effect. Three parameters of the BS model are the core radius, R_c, the softness parameter, a, and the valence Z. The value of R_c is generally fixed by fitting physical properties of the concerned systems [39]. We have taken the values of R_c for Al from Ref [18] [37]. The value for this is 1.91 au. Furthermore, at a core radius of R_c=1.91 au, e pair potential absence a local minimum; instead, it exhibits a principal minimum succeeded by Friedel oscillations [20]. This investigation was undertaken in order to avoid the local minimum

Table 1. Input parameters and calculated results.

Temperature, T (K)	Ionic number Density, ρ (Å^{-3})	Hard sphere diameter, σ (Å)	Packing fraction, Ω	Potential minimum (eV)	Valency, Z_s	Core radius, R_c (a.u.)	Softness parameter, a (a.u.)
950	5.314	2.80545	0.61437	−0.0011	3	1.91	0.49
1050	5.251	2.80245	0.60514	−0.00127	3	1.91	0.49
1150	5.189	2.80954	0.60255	−0.0014	3	1.91	0.49

effect of this R_c, which generates the effective potential pattern near −0.0011 eV. The softness parameter '*a*' is determined by the best fitting of the LWCA structure factor to the experimental ones. The values of '*a*' thus found for Al 0.49 au, respectively which is taken from our previous work [18] [37]. Regarding the third parameter called effective s-electron occupancy number, Z_s, we took the chemical valence 3 for Al. We note here that, the dielectric function plays an important role in determining the effective potential profile [20]. In this work we have used the dielectric function proposed by Icimaru and Utsumi [27], because of their theory satisfies the compressibility sum rule and the short-range correlation conditions for the wide range of metallic density as well avoid the local minimum.

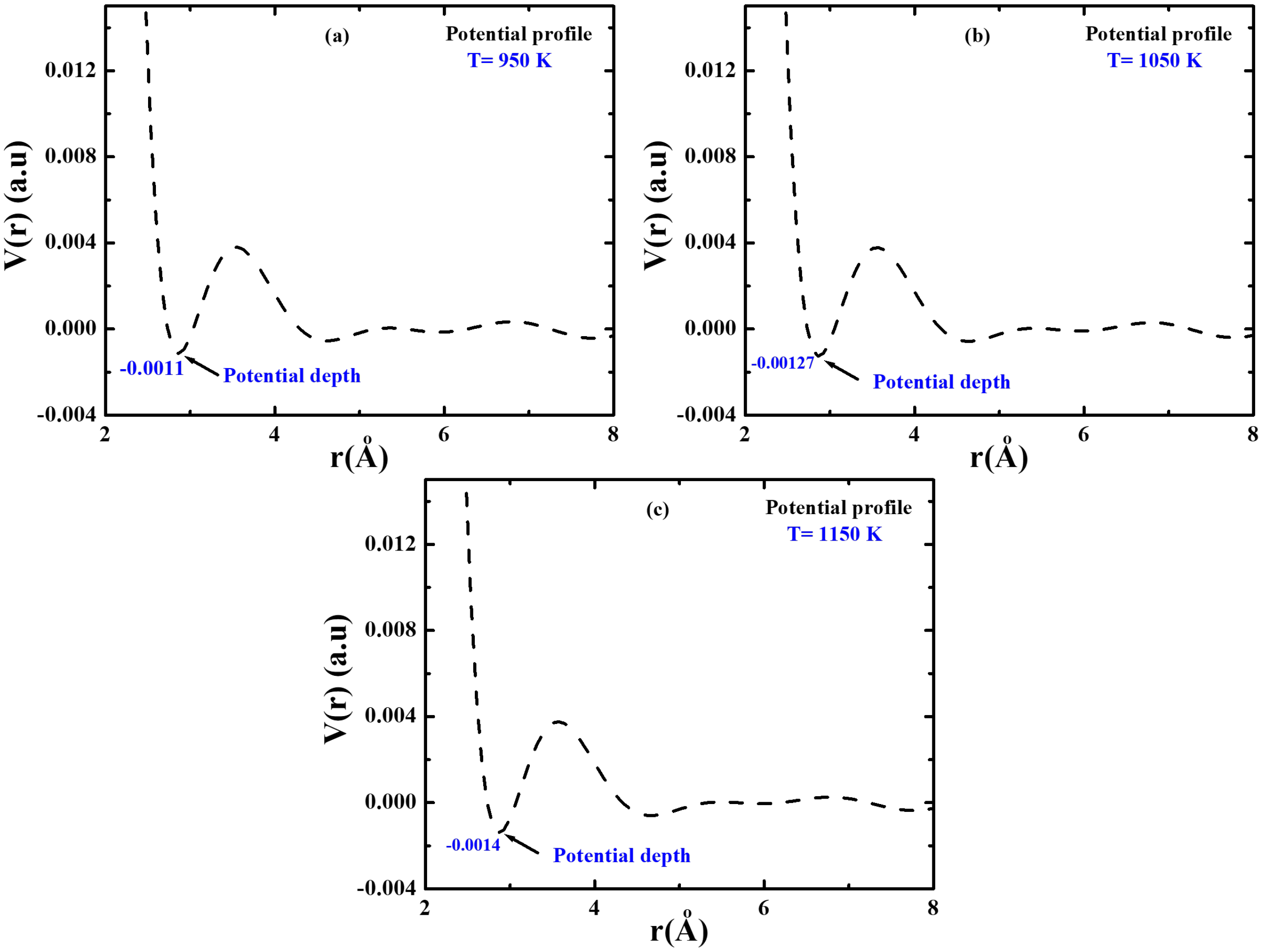

Figure 1. Pair potential profile for liquid Al at (a) 950 K, (b) 1050 K, and (c) 1150 K, respectively.

For calculating S_T and χ_T, we have used the relation in equations (6), and (7), sequential order. On the other hand, equation (8), and (9) employed for the estimation of η, and D. The major ingredients of the study of all the equations required are the packing fraction, Ω, and the temperature dependent effective HS diameter, $\sigma(T)$. We have ascertained them utilizing BS pseudopotential adjacent to LWCA perturbation theory.

Table 1 enumerates the input values that were subsequently obtained. We have applied to the LWCA theories of liquid structures to achieve them. The $\sigma(T)$ from LWCA is smaller than the one from an earlier study [18] [37] on Al-based alloys at a low temperature (973 K), because the $\sigma(T)$ in LWCA shows how far the origin is from the point where g(r) starts to be greater than zero. The graphical solution of the transcendental equation of equations used to estimate $S_T$is utilized to estimate $\sigma(T)$ for LWCA theory. Ω is then calculated from the relation, $\Omega = \pi\sigma^3 n/6$ [32]. Using these estimated values, the effective interionic interaction, $V(r)$, for the systems under consideration are calculated and shown in **Figure 1(a-c)**. According to the potential profile shown in **Figure 1**, the potential well's depth reaches its maximum at $T = 1150$ K. However, at 950 K, we have seen that the distance to the initial minimum reaches its lowest values. The depth of the well is determined by a subtle combined effect of the ionic density and the value of the valence of the metal. Besides, both repulsive and attractive forces must be exquisitely balanced to determine the potential well's depth. As a result, the potential well's depth varies from one metal to another and also showed a strong correlation

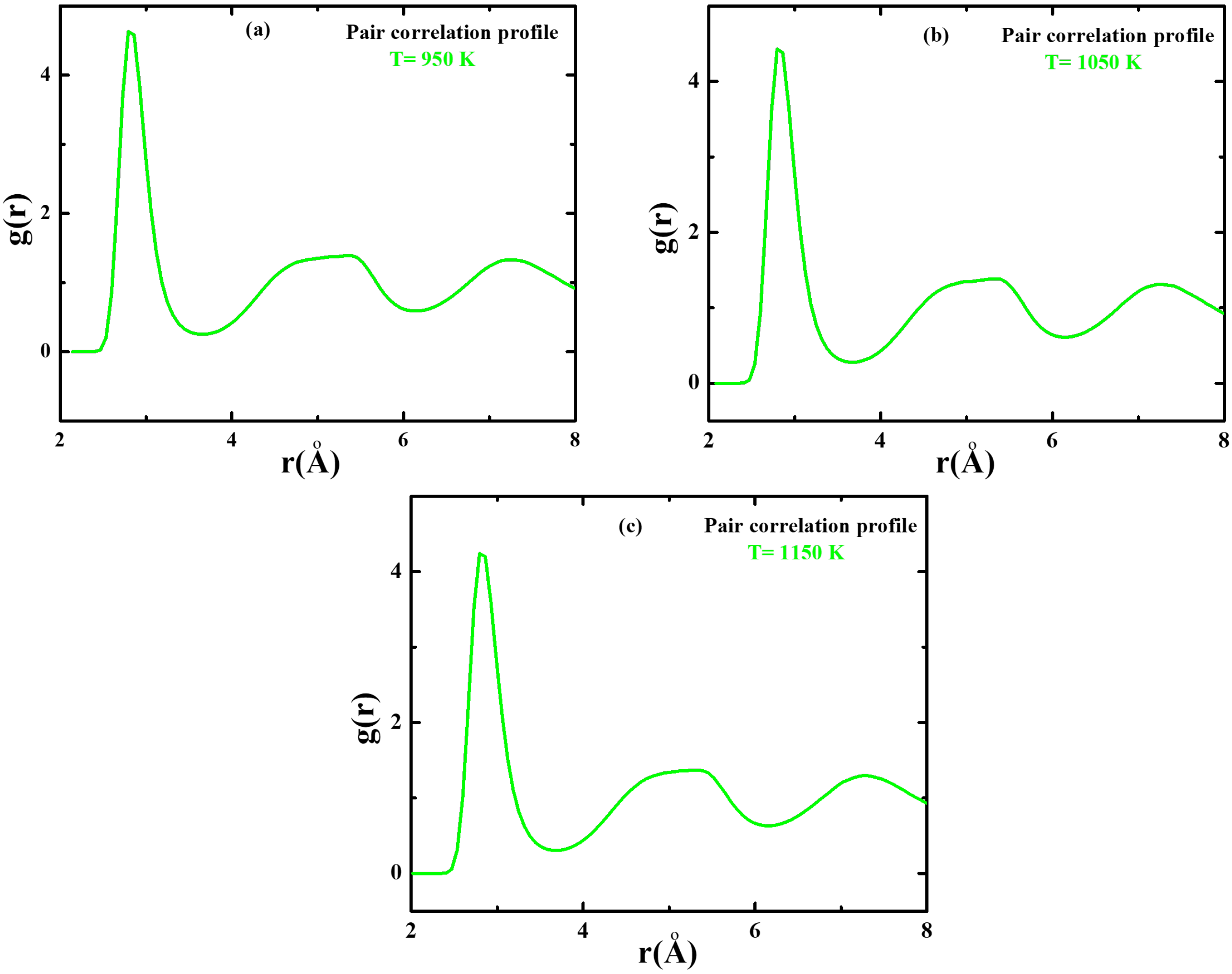

Figure 2. Partial pair correlation function for liquid Al at (a) 950 K, (b) 1050 K, and (c) 1150 K, respectively.

with varying parameters. A key factor in defining repulsive and attractive contributions to the interionic effective pair potential is the softness parameter, *a*. Moreover, in the present study consideration has been taken to avoid the local minima effect in the calculation to the principal minimum succeeded by Friedel oscillations. Perhaps this may be the reason for the potential well depth in the order of 10^{-4} (−0.0011eV). It is worth noting here that, the BS-model uses the empty core potential outside the core.

As can be seen in **Figure 2(a)-(c)**, temperature has an effect on pair correlation function. In this work, the pair correlation function, denoted by $g(r)$, of liquid aluminum is demonstrated at various temperatures. Besides we can see from **Figure 2(a)-(b)**, the height of the major peak reduces slightly as the temperature rises, while the peak position stays virtually the same. This observation has been noted previously [19] [20]. We found here that general agreement among g(r) for temperature fluctuations were better than the results obtained by previous researchers Bhuiyan *et al.* [19].

Figure 3(a)-(d) showed the χ_T, η, and D respectively. After comparing the present results of this study to experimental results, similar deviations have also been observed for them to the liquid polyvalent Al. It is believed that the same phenomena have also reflected for these microstructure properties. Besides, the uncertainty results for χ_T is 60%, on the other hand η, and D possesses 20% and 30 % respectively. Comparing among the investigated results to the sensitivity, it is found that the isothermal compressibility (χ_T) has the highest sensitive tendency which correlates electron density fluctuation has the significant impact on these properties. In addition, the calculated results for η, and D for the temperature range except for χ_T which has compared to the melting point experimental results demonstrated the similar tendency of decreasing (η), increasing (D) and increasing (χ_T) with the following temperature range for their corresponding experimental results [36]-[42]. However, in the present study, we have used microscopic theory involving perturbation scheme and the statistical mechanics. Here, three parameters R_c, a and Z_s are chosen only to calculate effective potentials. Once it is done, the rest of the calculations are completely parameter free. Moreover, calculations from the theoretical point of view are also self-consistent and, as a result the accuracy of calculations and the predictability of the theory is much more reliable than the empirical and semi-empirical methods. For each property measurement that was looked at, there is a difference between the experimental results and the estimated values because the same components and footing were used to get the results. Moreover, the deviation for χ_T was estimated as 10^{-2} order in range (**Figure 3(d)**). Furthermore, the uncertainty to sensitivity rearranges, then the studied properties can be found in the order, $\chi_T > D > \eta > S_T$.

Three possible manifestations of this divergence from the assessed results may arise. First, perhaps the underlying reason is that the BS potential has both an attraction and a repulsion component, LWCA theory only considers the repulsive portion of the potential profile derived from the BS pseudopotential. Overcoming

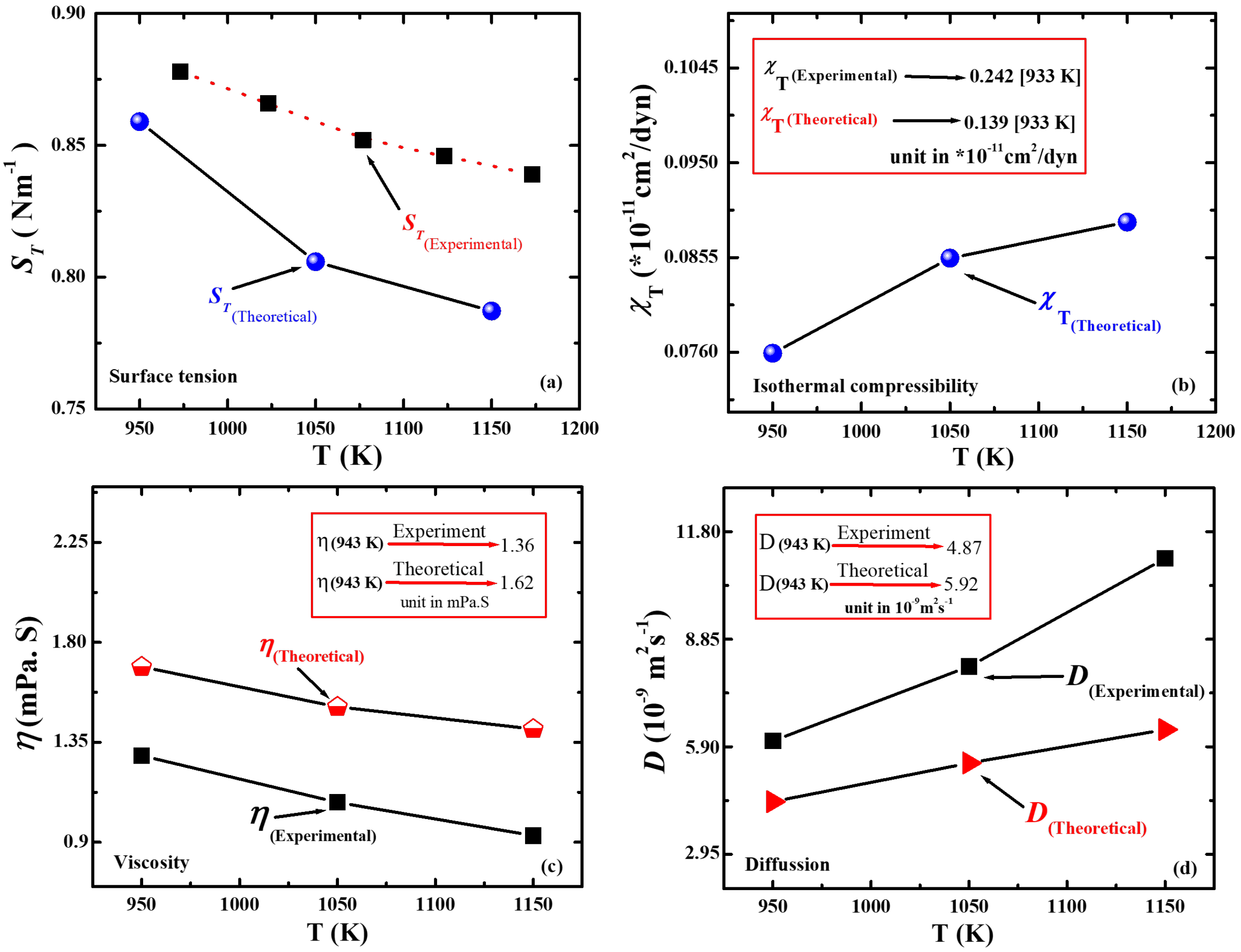

Figure 3. (a) Temperature dependence of Surface tension, S_T is plotted as a function of temperature for liquid Al. Square black color present the experimental results [1], and red circles present the calculated results for this study. Other calculated results are plotted in (b) isothermal compressibility (χ_T) [36], (c) shear viscosity (η) [41], and (d) diffusion coefficient (D) [42] for liquid Al. η and D compare with their melting temperature data.

the attractive part of the calculation could be the cause of this slight variation in the surface tension results. Second, the local field modifications suggested by Vashishta and Singwi (VS) [39] in the BS pseudopotential are crucial for obtaining an accurate assessment of the potential profile as illustrated in Figure 1(a)-(c). It (Figure 1(a)-(c)) reveals that the potential depth increases and the first minimum shifts marginally to the right, which correlates with the significance of local field correction in the pseudopotential analysis. So, the field correction is essential for authentic estimation. Third, there is a possibility bridization effect of liquid Al may occur, as demonstrated in Al cluster formation [43] [44]. In the literature [43] [44], it is mentioned that Al has hybridization effect as exhibited in Al Cluster. In addition, this study has been conducted the microstructural properties without considering the hybridization effect. Perhaps, if the hybridization effect may consider then there is a possibility to reduce the discrepancy between the present study and the experimental results.

The calculated values for physicochemical (S_T, χ_T,) and transport coefficients (η, D) are presented in this study. These properties are found to be deviated for the polyvalent liquid Al metallic element. A possible correlation between the hybridization effect and liquid Al was primarily confirmed [43]-[45]. Moreover, a strong connection shows the necessity of local field correlation in the pseudopotential application, which is significant for accurate estimation.

4. Conclusion

The findings of the S_T, χ_T, η, and D calculation for liquid aluminum are presented in this article. The temperature changes of the hard sphere diameter were assessed using the LWCA theory within the BS pseudopotential. Mayer's method has been utilized to calculate S_T for the liquid Al system across multiple temperature ranges. Carnahan and Stirling first order approximation was utilized for the mechanical profile evaluation as well χ_T. Sutherland *et al.* modification of the original Stokes-Einstein equation was employed for the estimation of η, and D. The result analysis suggested that the structure involving the full potential profile is significant for accurate numerical calculations. Moreover, a possible hybridization effect may also exist for the formation of the liquid Al structure. Further study is also needed to reveal the microstructural phenomenon of liquid Al.

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Conflicts of Interest

The authors of the study assert that there are no conflicts of interest.

Author Contributions

FIA: Conceptualization, Investigation, Writing-original draft, Plotting figures, Methodology, Software, review & editing, Supervision; S.C: Writing-Original, review & editing.

Data Availability

The raw/processed data required to reproduce these findings can be shared upon depending on request.

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