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Temperature Dependence of Schmidt Number of Composite Material Based Liquid Lithium

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Abstract

This work presents a simple formalism for Schmidt number and its temperature dependence for liquid lithium. It is explained that the temperature dependence of Schmidt number ($Sc = \eta/ \rho D$) can be understood through dependence of topological-short-range-order (TSRO) parameter on temperature. Expression for Schmidt number has been deduced in terms of average potential energy U_S of superficial core, probability of diffusional displacement (P) and the TSRO parameter (x) . Calculations have been made for liquid lithium across a broad range of temperature i.e. melting to boiling point. Highest deviation between calculated and experimental values is 9.2%,but in general deviations are within ±4.7% over the entire range. It is significant that derived equation for Schmidt number yields values that are not only in good agreement with experimental values over the liquid phase regime, but also predicts the expected values in corresponding temperature limits for the ideal gaseous phase ($x = 1$, D is large, so $Sc \rightarrow 1$) and ideal crystalline phase (as $x \rightarrow \infty$, $Sc \rightarrow \infty$).

Keywords: Composite material, Liquid theory, Schmidt number , Liquid lithium, Topological-short-range-order**)**

INTRODUCTION

Experimentally (X-ray and neutron diffraction studies) , it is established that atoms are correlated to each other up to few atomic diameters in the liquid phase [1,2]. Many theorist also stressed on existence of topological short-range – order (TSRO) in liquid metals [1,2]. But ,a very few attempts have been made to develop a formalism for the variation of TSRO parameter with temperature and its correlation with bulk properties [2] which may lead to a self- consistent and unified formalism for this state of matter. With this aim, author developed a statistical theory for liquid metal which has been used to study the temperature dependence of the TSRO parameter and a number of equilibrium and transport properties [3-8]. Applying the proposed theory, formalism for Schmidt number has been developed.

DEVELOPMENT OF THEORY

Temperature dependence of topological short-range order (TSRO)parameter

According to the proposed theory, liquid metal can be considered as a system containing of a huge number of ion – cores (nucleus and all inner electrons) and free electrons which are members of one or the other short-range-ordered regions. These regions are known as micro-regions. In these regions, ion-cores are correlated to each other through electric forces. At melting and higher temperatures, distance among atoms remains almost same as crystalline phase, therefore increase in bulk volume is distributed among micro-regions as a free space, these free space are known as micro – voids and enthalpy of fusion (L_m) is utilized

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in increase of surface energy due to conversion of long – range – order into short – range – ordered regions

$$L_m = dU = \sigma_m K \Delta S \quad . \tag{1}$$

dU is the total change in the internal energy of the system, σ_m is the free surface energy per unit area, K is a constant and it depends upon electronic configuration of the element and ΔS is the difference between the total surface area in the parent crystalline phase and the ensemble average surface area of all micro-regions in the liquid phase.A dimensionless parameter, $x = r / a$, Where "*r*" is the ensemble average size of the micro-region and $a = ((3V_S)/(4\pi N))^{1/3}$ is the radius of the area where a crystalline phase atom can exist just at the melting temperature. The TSRO parameter at the melting (x_m) can be obtained as

$$x_m \quad = \quad \left(\frac{4\pi V_S^2 N}{3}\right)^{1/3} \frac{\sigma_m K}{L_m} \tag{2}$$

Again above the melting temperature, the energy given to the system $\varDelta E_L$ can be expressed as the sum of increase in vibrational energy of ion-cores $\varDelta E_{vib}$, increase in diffusional energy of atoms $\varDelta E_{diff}$ and increase in energy of valence electrons $\varDelta E_{el}$ i.e. $\varDelta E_L = \varDelta E_{vib} + \varDelta E_{diff} + \varDelta E_{el}$.

The increase in the vibrational energy of the ion-cores ($\varDelta E_{vib}$) for rise in temperature $\varDelta T$ can now be written as

$$\varDelta E_{vib} \quad = \quad 3k_B N \left[1 - \frac{1}{x^3} + \frac{3T}{x^4} \cdot \frac{\varDelta x}{\varDelta T}\right] \varDelta T \tag{3}$$

$\varDelta E_{vib}$ is also related to increase in surface area as, $\varDelta E_{vib} = \sigma_m$ K $\varDelta$ *S* i.e.

$$\varDelta E_{vib} \quad = \quad -\frac{3\sigma_m K V_S}{a x^2} \varDelta x \tag{4}$$

From equations (3) and (4)

$$\int_{T_m}^{T} 3k_B N \left[1 - \frac{1}{x^3} + \frac{3T}{x^4} \frac{dx}{dT}\right] dT \quad = \quad -\int_{x_m}^{x} \frac{3\sigma_m K V_S}{a x^2} dx \tag{5}$$

Integrating and rearranging the terms, following expression is obtained for the TSRO parameter '*x*' [3]

$$\frac{1}{x^3} + \frac{4\pi\sigma_m K a^2}{3k_B T\, x} - \left[\left(1 - \frac{T_m}{T}\right) + \frac{T_m}{T}\left(\frac{1}{x_m^3}\right) + \frac{4\pi\sigma_m K a^2}{3k_B T\, x_m}\right] \quad = \quad 0 \tag{6}$$

The above equation can be solved by Cardano's formula. Its solution gives the variation of TSRO parameter (*x*) with temperature. Applying the proposed theory, expressions for various equilibrium properties viz. surface tension, excess entropy of melting, self-diffusion, viscosity, thermal conductivity, Schmidt number, Eucken factor, Prandtl number and specific heat at constant volume have been derived for inert liquids. These properties are calculated across a broad range of temperature from melting to critical temperature, there is a good agreement between experimental and calculated values [3,4]. Using the proposed theory, formalism for various properties viz. Surface tension ,excess entropy of melting, self-diffusion, viscosity, specific heat at constant volume have been derived for liquid metals. Calculations have been made across a broad range of temperature from melting to boiling temperature, agreement among experimental and calculated values is good [3-8]. In this paper, using the proposed formalism for self-diffusion and viscosity, expression for Schimt number has been derived and calculated for liquid lithium from melting to boiling temperature. Most of the calculated values are within the range of $\pm 4.7\%$,few calculated values are in the range of 7.3% - 9.2% with experimental values.

Temperature dependence of Self – diffusion Coefficient

According to proposed theory of liquid phase, probability for the diffusional displacement of a superficial atom per unit time P can be expressed as

$$P = \frac{1}{t_1 + t_2} = \frac{1}{\ell + a\exp\left(\bar{U}_S / k_B T\right)}\sqrt{\frac{8k_B T}{\pi m}} \quad (7)$$

Now, using above relations and following the well-known approach of kinetic theory, we can obtain an expression for the coefficient of self-diffusion *D* as explained below.

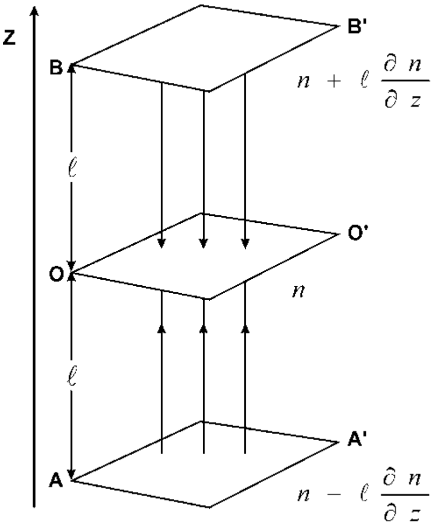

Figure1: Flux through the layers

Let us consider three parallel planes AA′, OO′ and BB′ at a distance ℓ from each other as shown in Figure1. Let the number density of atoms in the planes AA′, OO′ and BB′ be $(n - (\partial n/\partial z)\,\ell)$, n and $(n + (\partial n/\partial z)\,\ell)$ respectively. Since only superficial atoms n_s are contributing to the flux of mass, one should consider the number density of superficial atoms n_S, while writing the expression for mass flux. The number density of superficial atoms in layers AA′, OO′ and BB′ can be obtained as

$$n_{S_{AA'}} = \frac{4}{3}\frac{A}{x}\left(n - \frac{\partial n}{\partial z}\,\ell\right) \quad (8)$$

$$n_{S_{OO'}} = \frac{4}{3}\frac{An}{x} \quad (9)$$

And

$$n_{S_{BB'}} = \frac{4}{3}\frac{A}{x}\left(n + \frac{\partial n}{\partial z}\,\ell\right) \quad (10)$$

Here A is a constant, which depends on the surface to volume ratio of ordered micro-regions, which in turn would depend on electronic configuration of the elements. To obtain the atomic flux, the usual expression $(n\bar{v}/6)$ of kinetic theory must be replaced by (n_S P ℓ/6) since an atom remains attached to the surface for the finite time. The expression for atomic flux can be written as

$$J = \frac{P\ell}{6}\left[\frac{4}{3}\frac{A}{x}\left(n-\frac{\partial n}{\partial z}\ell\right)-\frac{4}{3}\frac{A}{x}\left(n+\frac{\partial n}{\partial z}\ell\right)\right]$$

Or

$$J = -\frac{4}{9}\frac{PA\ell^2}{x}\cdot\frac{\partial n}{\partial z} \tag{11}$$

Using equation (7) relation for J becomes

$$J = -\frac{4}{9}\left[\frac{1}{\ell + a\exp\left(\bar{U}_S/k_BT\right)}\sqrt{\frac{8k_BT}{\pi m}}\right]\cdot\frac{A\ell^2}{x}\cdot\frac{\partial n}{\partial z} \tag{12}$$

It is quite obvious from equation (12) that the liquid self-diffusion coefficient could be written as [5]

$$D = \frac{4}{9}A\frac{\ell^2}{x}\frac{1}{\left\{\ell + a\exp\left(\bar{U}_S/k_BT\right)\right\}}\cdot\sqrt{\frac{8k_BT}{\pi m}} \tag{13}$$

Equation (13) shows that the coefficient of self-diffusion dependence explicitly and implicitly (through ℓ and x) on temperature.

Viscosity and its temperature dependence

According to proposed theory, momentum is transferred by two types of motion (i) Diffusional motion. When the atoms diffuse from the surface of one micro-region in fast moving layer to the surface of another micro-region in slow moving layer (ii) Atomic correlation contribution: When the ion-cores move within the micro-region due to ion-ion interaction.

Diffusional Contribution

In figure 1, m ($u_x - (\partial u_x/\partial z)\,\ell$) , m$u_x$ and m ($u_x + (\partial u_x/\partial z)\,\ell$) are average momentum of atoms in the plane AA’,OO’ and BB’ respectively. Thus the net flux of momentum through layer OO’ can be written as

$$J_p = -\frac{4}{9}\frac{A}{x}nmP\ell^2\left(\frac{\partial u_x}{\partial z}\right) \tag{14}$$

Diffusional contribution to viscosity can be expressed as

$$\eta_d = \frac{4}{9}\rho\frac{A}{x}\frac{\ell^2}{\left(\ell + a\exp\left(\bar{U}_S/k_BT\right)\right)}\sqrt{\frac{8k_BT}{\pi m}} \tag{15}$$

Atomic correlation contribution

According to proposed model, any core which jumps in the micro-region, would impart a momentum mdu_x over an area πa^2 i.e.it would be proportional to x^2 ,Atomic correlation contribution can be written as

$$\eta_v \propto x^2 \tag{16}$$

Electrons also transfer momentum to ion-cores and this contribution can be expressed as

$$\eta_v \quad \propto \quad \left(B + \left(1 - e^{-(T - T_m)/T_m}\right)\right) \tag{17}$$

Here, B is a constant, combining equations (16) & (17)

$$\begin{aligned} \eta_v \quad &= \quad C_0 x^2 \left(B + \left(1 - e^{-(T - T_m)/T_m}\right)\right) \\ &= \quad C_0 B x^2 + C_0 \left(1 - e^{-(T - T_m)/T_m}\right) x^2 \end{aligned} \tag{18}$$

Viscosity of liquid metal can be written as

$$\square\square\square\square\square\square\square\square\square\square\square\square\square\square\square \ \square_{\square} \ \square\square_d \tag{19}$$

$$\eta = \rho D + C x^2 + C_0 (1 - e^{-(T-T)/T_{mm}}) x^2 \tag{20}$$

$$\begin{aligned} \eta \quad = \quad & C x^2 + \frac{4}{9} \rho \frac{A}{x} \frac{\ell^2}{\left(\ell + a \exp\left(\bar{U}_S / k_B T\right)\right)} \sqrt{\frac{8 k_B T}{\pi m}} \\ & + C_0 \left(1 - e^{-(T - T_m)/T_m}\right) x^2 \,. \end{aligned} \tag{21}$$

Schmidt number and its variation with temperature

Schmidt number Sc is the ratio of molecular diffusivity of momentum (η / ρ)to the molecular diffusivity of mass (D), i.e.

$$Sc \quad = \quad \frac{\eta}{\rho D} \,. \tag{22}$$

For ideal gas Schmidt number is one. Deviation from one show strength of the atomic correlations. Using equations (13), (20), and (22) the Schmidt number for liquid phase can be expressed as

$$Sc \quad = \quad 1 + \frac{C x^2}{\rho D} + \frac{C_0 \left(1 - e^{-(T - T_m)/T_m}\right) x^2}{\rho D} \,. \tag{23}$$

$$\begin{aligned} Sc \quad = \quad & 1 + \frac{C x^2}{\rho} \cdot \frac{9}{4} \cdot \frac{x}{A} \cdot \frac{\left(\ell + a \exp\left(\bar{U}_S / k_B T\right)\right)}{\ell^2} \left(\frac{\pi m}{8 k_B T}\right)^{1/2} \\ & + \frac{C_0 \left(1 - e^{-(T - T_m)/T_m}\right) x^2}{\rho} \cdot \frac{9}{4} \cdot \frac{x}{A} \cdot \frac{\left(\ell + a \exp\left(\bar{U}_S / k_B T\right)\right)}{\ell^2} \left(\frac{\pi m}{8 k_B T}\right)^{1/2} \,. \end{aligned} \tag{24}$$

From this equation it is obvious that Schmidt number for liquids would be much larger than one, i.e. in liquids due to the presence of TSRO parameter, momentum is transported more rapidly than the mass. Near melting *Sc* is expected to have large values (as it should be approximately infinity for ideal crystalline phase). With rise in temperature as *x* decreases and *D* increases, *Sc* is expected to decrease. Equation (24) along with equation (6) gives the exact functional dependence of Schmidt number on temperature.

RESULTS AND DISCUSSION

The input parameter ρ have been taken from literature [9]. Same values of TSRO parameter is used in calculation of self-diffusion, viscosity and other properties of liquid lithium [3-8]. Values of *A, US ,C,* C_0 are mention in table1 . These values are also used in the calculations of self-diffusion coefficient for liquid lithium. Deviations between experimental and calculated values are within 5.7% for self-diffusion of liquid lithium (The paper entitled "A theoretical study of viscosity for liquid lithium and its temperature dependence” has been communicated to Material Science Forum). Using the equation (23), viscosity of liquid lithium has been calculated over a wide range of temperature from melting to boiling temperature. The maximum difference between calculated and experimental data for liquid lithium is 6.6%, a value that falls comfortably within the bounds of experimental uncertainty.

The calculated values of *Sc* along with the available experimental data [10,11,12] of *Sc* have been reported in Table (2) which shows a quite fair agreement, the maximum deviation is 9.2%. These have also been plotted in Figures (2). In our earlier work formalism for Schmidt number of inert liquids has been developed [8]. It is found that the value of Schmidt number for inert liquids at the melting temperature is around 100 which decrease gradually with rise in temperature to around 10 near critical temperature. Whereas in case of metallic liquids, it is around 200 at melting temperature, it goes to around 9 at boiling temperature. This clearly reflects the trends of Schmidt number. It is interesting to see that equation (21) gives not only the values in good agreement with experimental values over liquid phase regime, but it also predicts the expected values for ideal crystalline phase (as $x \to \infty$, $Sc \to \infty$) and ideal gaseous phase ($x = 1$ and *D* is large so $Sc \to 1$) in corresponding temperature limits. In fact, Schmidt number shows the relative ease with which momentum is transported to the ease with which particle is transported. It is a measure of atomic correlations. Hence fall in *Sc* reflects clearly the loss in TSRO parameter. Thus, the trends of *Sc* versus *T* are in conformity with proposed model for the liquid phase. Figure (2) clearly reflect the above-mentioned aspects.

Table 1. Values of various constants for liquids lithium.

Element	*A*	US x10^{19} (J)	$C \times 10^5$ (kg m^{-1} s^{-1})	$C0 \times 10^5$ (kg m^{-1} s^{-1})
Lithium	0.5	2.64	1.37	6.86

Table2. Comparison of experimental and present calculated values of Schmidt number ‘*Sc*’ for liquid lithium.

T (K)	$Sc_{exptl.}$	***x***	$\eta_{calcd.}$ **× 10^5 (kg m^{-1} s^{-1})**	$D_{calcd.}$ **× 10^9 (m^2 s^{-1})**	$Sc_{calcd.}$ **(% Dev.)**
454	197.74	6.31	55.09	5.61	189.18 (-4.3)
500	139.48	5.09	53.25	7.76	134.00 (-3.9)
550	101.18	4.23	48.55	9.47	101.08 (-0.1)
600	77.40	3.64	43.82	11.11	78.58 (1.5)
650	61.52	3.21	39.62	12.71	62.72 (1.9)
700	50.34	2.89	36.18	14.29	51.45 (2.2)
750	42.15	2.64	33.28	15.88	43.03 (2.1)
800	35.95	2.44	30.83	17.47	36.61 (1.8)
850	31.13	2.28	28.82	19.07	31.68 (1.8)
900	27.31	2.15	27.18	20.69	27.83 (1.9)
950	24.22	2.04	25.75	22.33	24.68 (1.9)
1000	21.68	1.95	24.59	24.00	22.18 (2.3)
1050	19.57	1.87	23.52	25.68	20.04 (2.4)
1100	17.79	1.80	22.57	27.39	18.23 (2.5)
1150	16.27	1.75	21.99	29.12	16.89 (3.8)
1200	14.97	1.70	21.33	30.88	15.63 (4.4)

1250	13.88	1.65	20.61	32.66	14.47 (4.2)
1300	12.90	1.61	20.07	34.46	13.51 (4.7)
1350	12.04	1.57	19.73	36.29	12.76 (6.0)
1400	11.27	1.55	19.11	38.14	11.90 (5.6)
1450	10.60	1.57	18.92	40.02	11.37 (7.3)
1500	10.00	1.49	18.48	41.92	10.73 (7.3)
1550	9.46	1.47	18.25	43.85	10.25 (8.3)
1600	8.97	1.45	17.99	45.81	9.80 (9.2)
1620	8.79	1.44	17.84	46.60	9.60 (9.2)

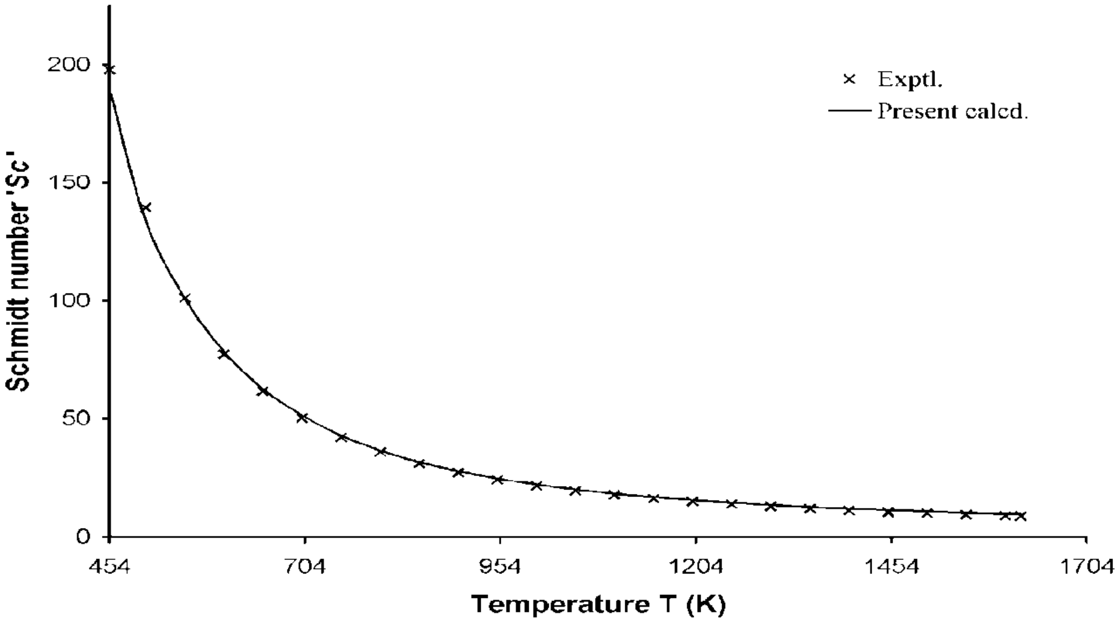

Figure 2. Variation of Schmidt number Sc with temperature T for liquid lithium.

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