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Theoretical Study of Electrical Transport Properties of Some Simple Liquid Metals by Pseudopotential

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ABSTRACT

Here electrical transport properties to be particular, electrical resistivity (ρ_l), thermoelectric power (TP) and thermal conductivity (σ_l)has been reported by us of some basic liquid metals i.e. Na, Mg, Al, Pb of various gatherings (Z=1 to Z=4) of occasional table based on display potential formalism. The outstanding all inclusive capability of Fiolhais et al. is utilized out of the blue with five unique sorts of nearby field remedy work given by Hartree (HR), Taylor (TY), Ichimaru-Utsumi (I&U), Farid et al. (FR) and Sarkar et al. (SR) in the present calculation and discovered appropriate for each examination. The generalized mean spherical approximation (GMSA) technique is embraced for processing the structure factor of liquid metals. The by and by acquired outcomes are contrasted and the other such information either hypothetical or exploratory wherever exist in the writing and discovered fruitful.

KEY WORDS: Pseudopotential, GMSA structure factor, Electronic Transport Properties, Liquid metals

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INTRODUCTION

Liquid metals, specifically the mono nuclear ones, have been perceived since long prior to be the model of basic liquids, as they incorporate a large portion of the physical properties of genuine liquids without the confusions which might be available in a specific framework [1]. Not with standing that, metallic liquids, for example, liquid sodium, having comparative thickness and consistency to water, discover application as coolant in atomic reactors. For these reasons, current enthusiasm of work is centered on the non-crystalline frameworks i.e. liquid metals [1].

Liquid metals can be depicted as mixes of electrons and particles. A part of the electrons (the middle electrons) remain nearby centers and are incidentally impacted by the atomic development. Whatever remains of the electrons (valence electrons) are flexible through social gathering of particles and are accountable for the vehicle and moreover solid properties of the liquid metals [2].

In the present work, the electrical transport properties reported by us such as electrical resistivity (ρ_l), thermoelectric power (TP) and thermal conductivity (σ_l) of some simple liquid metals with the help of pseudopotential theory. A well-known universal model potential proposed by Fiolhais et al. [3] used to describe the electron-ion interaction in these system is of the form

$$V(r) = -\frac{Z}{R}\left\{\frac{1}{x}\left[1-(1+\beta x)e^{-\alpha x}\right]-Ae^{-x}\right\} \tag{1}$$

Other details of this potential are described in the paper of Fiolhais and co-workers [3].

In the midst of the latest a significant extended period of time there has been a creating focus in the properties of liquid metals and their amalgams. It demonstrates metallic and liquid like lead and thusly can make a connection between the theory of the liquid states and the speculation of the electronic states in metals and in this manner the examination of electrical transport properties of liquid metals and their composites remain a champion among the most respected properties either likely or theoretically [4-27].

The Free electron (NFE) hypothesis proposed by Ziman [8, 9] has been genuinely beneficial in delineating the quantitative direct of the electrical properties of liquid metals. Since in these metals the mean free way is about the one hundred times the interatomic discrete and the slight scrambling picture ought to be liberal. Promote more for the liberal polyvalent metals where the meanfree way is simply around two interatomic detachments consequently such model can make theoretical results, which are sensible in simultaneousness with the trial one. In the present calculation of electrical resistivity (ρ_l), thermoelectric power (TP) and thermalconductivity (σ_l) of liquid metals, the nearby field revision works because of Hartree (HR), Taylor (TY), Ichimaru-Utsumi (I&U), Farid et al. (FR) and Sarkar et al. (SR) [15] are utilized to examine the impact of trade and relationship impacts. The generalized mean spherical approximation (GMSA) strategy [28] is received for figuring the hypothetical structure factor of liquid metals in the present calculation.

METHOD OF COMPUTATION

The well-known book of Faber [7] explains us electrical resistivity (ρ_l) of liquid metals expect the model of a gas of conduction electrons which cooperate with and are scattered by unpredictably put metal particles. Tolerating the free-electron arrangement, a clarification for the electrical resistivity (ρ_l) of liquid metal the degree that the commonplace of the consequence of the structure factor and pseudopotential cross section segment is made as [4-27].

$$\rho_l = \frac{3\pi m^2}{4e^2\hbar^3 n k_F^6}\int_0^\infty S(q)|V(q)|^2 q^3\, dq\, \theta(2k_F - q). \qquad (2)$$

Where n the electron thickness is identified with Fermi wave number and θ is the unit step work that cuts of the q - incorporation at $2k_F$ comparing to a splendidly sharp Fermi surface, $S(q)$ the structure factor and $V(q)$ the screened particle pseudopotential shape factor. Here, we have Generalized Mean Spherical Approximation (GMSA) definitions [28] for producing the structure factor S(q) of the metallic components.

The articulation for thermoelectric power (TP) is given by, [4, 5]

$$TP = -\left(\frac{\pi^2 k_B{}^2 T}{3|e|E}\chi\right)\Bigg|_{E=E_F} \qquad (3)$$

where,

$$\chi = 3 - \frac{2S(2k_F)V^2(2k_F)}{\left\langle S(q)|V(q)^2|\right\rangle} \qquad (4)$$

Where, $V(q)$ is the screened ion potential, S(q) is the structure factor, $2k_F$ corresponding to a perfectly sharp Fermi surface.

We understand that, if a temperature incline is related with a metal, the conduction electrons will pass on a gleam current along it regardless of the way that an electric current is kept from gushing and that point of fact they are responsible for the immense piece of the warm conductivity. The clarification for thermal conductivity (σ_l) for liquid metals can be made as [4, 5].

$$\sigma_l = \frac{\pi^2 k_B{}^2 T}{3e^2\rho} \qquad (5)$$

RESULTS AND DISCUSSION

The input parameters and constants used in the present computations are written in Table-1, which are taken directly from [3]. Here we are considered universal parameters of the model potential.

Table No. 1Input parameters and constants

Metal	Z	Ω(au)	T(K)	η	α(U)*	R(U)*
Na	1	254.25	378	0.46	3.075	0.528
Mg	2	155.90	1053	0.46	3.502	0.382
Al	3	111.46	1043	0.45	3.635	0.334
Pb	4	203.86	713	0.43	3.337	0.466

* U-Universal Parameters

The by and by figured aftereffects of electrical transport properties of liquid metals are described in Table 2-4 with accessible exploratory [5, 7, 16, 25] or hypothetical information [5-7, 11-27] wherever exists in writing.

Table No. 2Electrical Resistivity (ρ_l) (in $\mu\Omega - cm$) of liquid metals

Metals	Present results					Expt. [5, 7, 16, 25]	Others [5-7, 11-27]
	HR	TY	I&U	FR	SR		
Na	8.52	15.63	17.14	17.38	12.58	9.6	5.3,7.9, 8.44, 9.48, 9.82, 10.11,10.25,10.38,13.58, 13.91, 15.8, 16.3, 18.50, 17.24, 37.7
Mg	10.65	16.53	17.12	17.49	13.645	26	16.42, 17.3, 23.7, 23.79, 27.02,28.02,29.13,29.75, 30.28,32.41,37.93,38.98, 40.12, 59.08
Al	23.68	34.78	36.08	36.37	28.00	24	12.17,20.8, 20.76, 21.65, 22.21,24.02,25.28,26.77, 27, 34.12
Pb	46.70	72.16	75.98	77.56	57.85	95	57.46, 64, 68.9, 79.13, 90.59,94.16,94.57,96.64, 110.33, 121, 129.16

It is similarly observed from Table 2 that, the present eventual outcomes of the electrical resistivity (ρ_l) of the liquid metals are found in subjective concurrence with the test [5, 7, 16, 25] or theoretical [5-7, 11-27] revelations. Also, it is seen that, among the five utilized close-by recorded survey works, the territory field modification work because of HR (without trade and affiliation) gives the base numerical estimation of the electrical resistivity, while the zone field amendment work on account of FR gives the most outrageous regard. In connection with the eventually enrolled outcomes of the electrical resistivity (ρ_l) from static HR-work, the percentile impacts for Na, Mg, Al and Pb liquid metals of TY, I&U, FR and SR-limits are of the request 47.68% - 104.04%, 28.06% - 64.12%, 18.22% - 55.69% and 23.88% - 66.08%, exclusively.

Table No. 3 Thermoelectric power *(TP) (* in μVK) of liquid metals

Metals	Present results					Expt. [5, 7, 16, 25]	Others [5-7, 11-27]
	HR	TY	I&U	FR	SR		
Na	-8.21	-8.21	-8.25	-8.24	-8.23	-9.90	-8.67,-8.75, -8.76,-8.93
Mg	-7.02	-7.06	-7.33	-7.25	-7.20	-	-6.35, -6.52, -6.59, 4.93, 5.88, 1.6
Al	-5.00	-5.07	-5.17	-5.15	-5.07	-2.10	-0.40, -0.87, -4.75,-4.82, -4.83, -4.85, -4.90, -4.93
Pb	-4.46	-4.52	-4.60	-4.59	-4.52	0.71	-4.86,-4.86,10.32,-10.52,-10.64,-10.58,-10.85,-10.92, 2.6

From Table it is seen that five used neighborhood field review work, the close-by field cure work in view of HR (without trade and affiliation) gives the base numerical estimation of the TP, while the territory field change work because of FR gives the most extraordinary regard. The percentile impacts from static HR-chip away at the TP for Na, Mg, Al and Pb liquid metals of neighborhood field amendment limits are found of the demand of 0.09% - 0.47%, 0.64% - 4.42%, 1.41% - 3.38% and 1.39% - 3.27%, independently. The present results are found comparative with open trial [5, 7, 16, 25] and speculative [5-7, 11-27] information.

Table No. 4 Thermal conductivity (σ_l) (in $watt\ K^{-1}cm^{-1}$) of liquid metals

Metals	Present results					Others [5-7, 11-27]
	HR	TY	I&U	FR	SR	
Na	1.08	0.59	0.54	0.53	0.73	0.205, 2.2
Mg	2.41	1.56	1.50	1.47	1.88	0.0231
Al	1.08	0.73	0.71	0.69	0.91	0.24, 2.4
Pb	0.37	0.24	0.23	0.22	0.30	0.039, 2.4

From Table 4 we can see that among the five used neighborhood field amendment works, the close-by field review work due to FR gives the base numerical estimation of warm conductivity (σ_l), while the adjoining field adjustment work HR (without trade and relationship) gives the most outrageous regard. In examination with the before long handled eventual outcomes of the thermal conductivity (σ_l) from static HR-work, the percentile impacts for Na, Mg, Al and Pbliquid metals of different nearby field remedy capacities are of the request of 32.29% - 50.99%, 21.91% - 39.07%, 15.41% - 35.77% and 19.26% - 39.79% individually. The trial data of thermal conductivity isn't open in the written work however the relationship amongst's before long handled data and others yielding [5-7, 11-27] are seen comparable.

The impact of nearby field adjustment capacities assumes an essential part in the calculation of electrical transport properties of the liquid metals. The nearby field redress works because of I&U, FR and SR can produce stable outcomes with respect to the electrical transport properties of the liquid metals of the diverse gatherings of the intermittent table as those acquired from all the more normally utilized HR-and TR-neighborhood field rectification capacities. Therefore, the utilization of these more positive nearby field remedy capacities is built up effectively.

CONCLUSIONS

In conclusion we reason that, the present calculations not only confirm the appropriateness of all inclusive model capability of Fiolhais et al. for concentrate previously mentioned properties yet it additionally builds up the utilization of more noticeable dielectric capacities.

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