JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **11** No 1, 01004(4pp) (2019)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **11** № 1, 01004(4cc) (2019)

Electrical Transport Properties of Liquid $Li_{1-x}Na_x$ Alloys

R.C. Malan[1,*], A.M. Vora[2,†]

[1] *Applied Science and Humanities Department, Government Engineering College, (G. T. U.), Valsad-396001, Gujarat, India*
[2] *Department of Physics, University School of Sciences, Gujarat University, Ahmedabad-380009, Gujarat, India*

(Received 01 December 2018; revised manuscript received 03 February 2019; published online 25 February 2019)

Metals, being a less resistive to the flow of electrons, have been used for electrical conduction since the beginning. The factors affecting this flow have always been a focus of researchers working in this field. With the development of material science and the condensed matter physics, a high degree of accurate prediction for the electron behavior in the solid phase of the metals becomes possible. However, the liquid state is more unpredictable in metals as well as in alloys. Electron flow and hence the other properties of the sample as a whole will get change when two or more metals are combined to get form of alloys. It will be interesting to mathematically model the electrical transport in the metals and alloys, particularly in the liquid state. Alkali metals have their own importance in the field of the nuclear reactors. Lithium as having large absorption cross section is used for the coolant in many types of reactors. The small amount of electron current may in turn be converted in the cyclic heating and hence the raise in the temperature of the coolant itself. In present work, an effort has been made to check the electrical transport in liquid binary alkali alloy of lithium with sodium at different proportions. Some important electrical transport properties of the liquid $Li_{1-x}Na_x$ binary alloys have been reported with the help of classical pseudopotential theory. The study includes the investigation of the electrical resistivity, the thermoelectric power and the thermal conductivity of the said alloy using a universal model potential of Fiolhais *et al.* for the first time to the best of our knowledge. Variety of the local field correction functions (starting from a static dielectric function given by Hartree (H) to the exchange and correlation functions given by Hubbard-Sham (HS), Taylor (T), Vashishta-Singwi (VS), Farid *et al.* (F), Ichimaru-Utsumi (IU), Nagy (N) including recent one given by Sarkar *et al.* (S)) are employed in the present computations and found appropriate for such a study. The presently computed values of the electrical resistivity agree reasonably well with the experimental data.

Keywords: Electrical resistivity, Pseudopotential theory, Liquid alkali alloys.

DOI: 10.21272/jnep.11(1).01004 PACS number: 72.15.cz

1. INTRODUCTION

Apart from the solid state of matter, researchers are interested in various types of study of the liquid phase of metals and their mixtures. Because of the presence of conduction electrons and the available range of interparticle distance in a molten state, it shows a modified metallic type of behaviour and it correlates the concept of a molten state with those of electronic states in metallic elements. Therefore, the experimental, as well as the theoretical study of such electrical properties of liquid metals and their various mixtures in the form of alloys are having their own importance till today. There exist a large number of studies reported for studying the electrical properties of liquid metals or their alloys using various well-known pseudopotentials with the conventional dielectric screening functions [1-5].

In the present article, the three electrical transport properties, such as the electrical resistivity (ρ_{alloy}), the thermoelectric power (TEP_{alloy}) and the thermal conductivity (σ_{alloy}) of $Li_{1-x}Na_x$ binary alloys are investigated with the help of universal model potential proposed by Fiolhais *et al.* [6]. The pseudopotential theory has its own importance and advantages over the other complicated methods. Selection of the said potential [6] is made due to its high ability to produce the results for many of the properties of liquid alkali metals as well as alloys. The quality of the results obtained for the electrical and thermodynamic properties reported in our previous articles [2-3] are the motivation for present investigation.

The proportion of each element present in the given binary mixture plays an important role to decide the said electrical properties. This type of study is possible with the help of the approach given by Faber-Ziman [1, 3, 5]. Various local field correction functions proposed by Hubbard-Sham (HS), Vashishta-Singwi (VS), Taylor (T), Ichimaru-Utsumi (IU), Farid *et al.* (F), Sarkar *et al.* (S) and Nagy (N) [2-4] are used to examine the influence of screening with respect to the static Hartree (H)-function.

2. COMPUTATIONAL METHODOLOGY

The computation of ρ_{alloy} is carried out with the help of the analytical expression for alloys proposed by Faber and Ziman [1, 3, 5]

$$\rho_{alloy} = \frac{12\Omega_0}{k_F^2}\int_0^{2k_F}\left[(1-x)a_{11}(q)W_{11}^2 + xa_{22}(q)W_{22}^2 + 2\sqrt{x(1-x)}a_{12}W_{11}^2(q)W_{22}^2(q)\right]qdq, \quad (1)$$

* rcmgecv@gmail.com
† voraam@gmail.com

where $W_{11}(q)$ and $W_{22}(q)$ represent the form factors of the model pseudopotential for the two metals 1 and 2. The partial structure factors of Ashcroft-Lengreth are denoted by a_{ij} [4], while x is the concentration of the second metallic component.

The structure factor and potential dependent TEP_{alloy} can be expressed as follows [1, 3, 5]

$$TEP_{alloy} = -\left[\frac{-0.001795T(3-2\lambda(q)q)}{E_F}\right]. \quad (2)$$

Instead of the physical flow of the electrons, only the heat can pass through the metal by applying the temperature gradient to the liquid. The rate of this heat flow for a given liquid is a measurement of σ_{alloy}. It can be written as follows [1, 3, 5]

$$\sigma_{alloy} = \left(\frac{\pi^2 k_B^2 T}{3|e|^2 \rho_{alloy}}\right). \quad (3)$$

Here e, E_F, T and k_B are the electronic charge, Fermi energy, temperature and the Boltzmann's constant, respectively. The universal model potential of Fiolhais *et al.* [6] is used in the present computation in the following form [6]:

$$W(q) = \frac{8\pi ZR^2}{\Omega_0 \varepsilon(q)}\left[-\frac{1}{(qR)^2} + \frac{1}{\left[(qR)^2+\alpha^2\right]} + \frac{2\alpha\beta}{\left[(qR)^2+\alpha^2\right]^2} + \frac{2A}{\left[(qR)^2+1\right]^2}\right], \quad (4)$$

where R is the core decay length. The two parameters A and β are determined from the analytical conditions i.e. $r = 0$ and discussed in [6]. Also, Z, Z and $\varepsilon(q)$ are the valence, the atomic volume and the modified Hartree dielectric function, respectively. The screening influences are studied by using eight different local field correction functions given by various authors used in the present computation for the very first time with this universal model potential.

3. RESULTS AND DISCUSSION

The required inputs used in the present calculations are shown in Table 1, which are adopted directly from [6]. The present results of various electrical transport properties are displayed in Figs. 1-3.

Table 1 – The input parameters and constants

Metal	Z	Z, a.u.	η	α, a.u. [6]	R, a.u. [6]
Li	1	142.47	0.46	3.546	0.361
Na	1	254.25	0.46	3.047	0.528

The concentration dependence ρ_{alloy} of $Li_{1-x}Na_x$ binary alloys is shown in Fig. 1 with available experimental data [7]. From Fig. 1, it can be observed that the present results for ρ_{alloy} due to VS-function are found to be in good agreement with the experimental data [7]. The relative influence of all the functions with respect to static H-function on the results of ρ_{alloy} is found in the range of 22.28 %-141.57 %.

While the presently computed results of TEP_{alloy} of $Li_{1-x}Na_x$ binary alloys are displayed in the Fig. 2.

It can be easily noted that among all eight employed local filed correction functions in the present work, the results of H-function show the maximum numerical value of TEP_{alloy}, while those due to N-function give the minimum value. Also, the presently obtained results for σ_{alloy} of said binary alloys are illustrated in Fig. 3.

It is observed that the present results of σ_{alloy} computed through H-function show higher results while N-function produces lower values in comparison with other local field correction functions. As per literature survey done prior to this work, the experimental information regarding TEP_{alloy} and σ_{alloy} at each of the concentration (x) values are not available for further

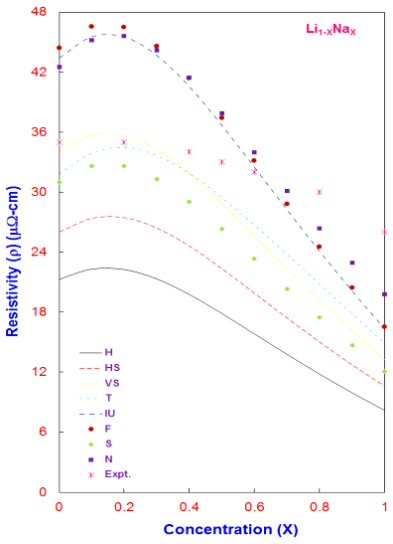

Fig. 1 – ρ_{alloy} of $Li_{1-x}Na_x$ binary alloys

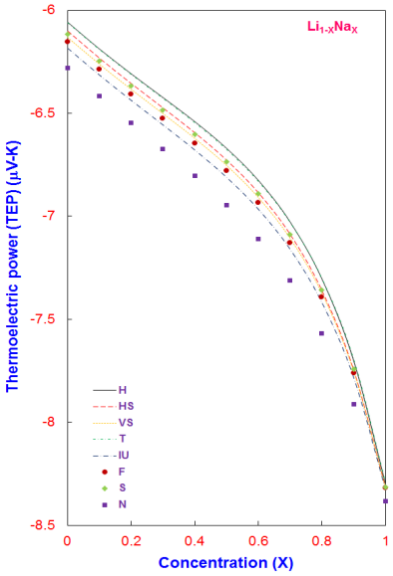

Fig. 2 – TEP_{alloy} of $Li_{1-x}Na_x$ binary alloys

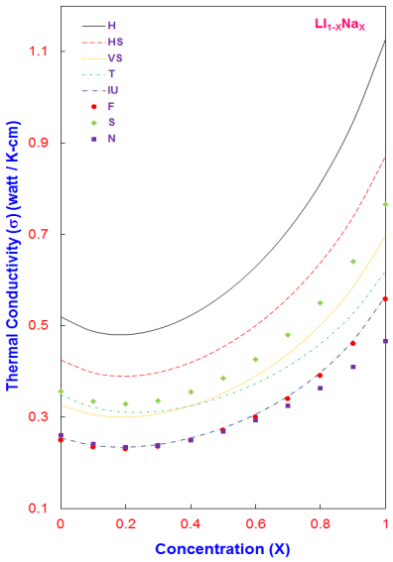

Fig. 3 – σ_{alloy} of $Li_{1-x}Na_x$ binary alloys

comparison, and hence because of the lake of experimental data these types of calculations may become very important and can be considered as one of the procedures for further examinations of the materials.

3.1 Physical significance of the results

The parabolic shape obtained for curves of ρ_{alloy} and σ_{alloy} shows the agreement of the present results and the previous results obtained by Vora [8]. According to the present result, if the binary alloy of Li and Na is formed with concentration $x = 0.2$, then the maximum ρ_{alloy} can be obtained. Peak is not found at exactly mid of the concentration as in the case of Vora [8]. Thus, the present potential provides better agreement than the results presented in [8]. Compared to the results generated by self-consistent approach reported by Geertsma *et al.* [9], present peak in the resistivity holds a better position with respect to the experimental results referenced in [9]. As lithium being an important element in nuclear reactors, it is worth to find this type of very sensitive transport properties [10]. Many of the researchers have skipped Li as well as the alloys consisting Li from their study, due to various computational and theoretical limitations to generate the reliable results. Hence the current results fill the gap by selecting Li in the study. This happens due to change in the electronic configuration of both participating elements for the formation of the alloy. Further, to increase ρ_{alloy} the concentration proportion of Na is to be increased. This prediction becomes more important while using the mixtures as the intermediate liquid layers in the nuclear reactors. As even a small amount of the current flow can give rise to the increase in the temperature which may convert in the cyclic current and heat increased in the whole fluid as well. As the present work involves only directly adopted set of the universal potential parameters (without any kind of modification) given by Fiolhais *et al.* [6], there is a scope of getting more improved results than the presently achieved findings. This can be done either by adopting other forms of local field correction functions or by developing a bit modified method for potential parameter determination. The reported work confirms the applicability of the universal model potential of Fiolhais *et al.* [6] in the afore mentioned properties of liquid $Li_{1-x}Na_x$ binary alloys along with all the used local field correction functions and found successful.

4. CONCLUSIONS

Looking at the overall picture of the presently computed results, it can be stated that the study not only supports the reliability of the universal model potential of Fiolhais *et al.* [6] for investigating the aforesaid electronic properties of $Li_{1-X}Na_X$ liquid binary alloys, but it also suggests appropriate selection and use of more promising local field correction functions in the present study of binary mixtures.

REFERENCES

1. S. Korkmaz, S.D. Korkmaz, *Int. J Thermo. Phys.* **33**, 831 (2012).
2. R.C. Malan, A.M. Vora, *J. Nano-Electron. Phys.* **10**, 03020 (2018).
3. R.C. Malan, A.M. Vora, *Int. J. Sci. Res. Rev.***7**, 385 (2018).
4. A.M. Vora, *Int. Lett. Che. Phys. Astro.* **54**, 56 (2015).
5. S.D. Korkmaz, S. Korkmaz, *J. Mol. Liq.***186**, 85 (2013).
6. C. Fiolhais, J. Predew, S.Q. Armster, J.M. McLaren, M. Brajczewska, *Phys. Rev. B* **51**, 14001 (1995).
7. P.D. Feitsma, J.J. Hallers, F.V.D. Werff, W. Van Der Lugt, *Physca B+C* **79**, 35 (1975).
8. A.M. Vora, *Tur. J. Phys.* **31**, 341 (2001).
9. W. Geertsma, D. Gonzalez, L.H. Gonzalez, *Braz. J. Phys.* **33**, 408 (2003).
10. M.S. El-Genk, J.M. Tounier, *J. Nucl. Mater.* **340**, 93 (2005).

Електричні транспортні властивості рідких сплавів $Li_{1-x}Na_x$

R.C. Malan[1], A.M. Vora[2]

[1] *Applied Science and Humanities Department, Government Engineering College, (G. T. U.), Valsad-396001, Gujarat, India*
[2] *Department of Physics, University School of Sciences, Gujarat University, Ahmedabad-380009, Gujarat, India*

Метали із відносно малим питомим опором використовуються дуже давно. Фактори, що впливають на питомий опір, завжди були предметом аналізу дослідників цієї галузі. З розвитком матеріалознавства і фізики конденсованих матеріалів став можливим високий рівень точного прогнозування поведінки електронів у твердій фазі металів. Однак, рідкий стан є більш непередбачуваним як в металах, так і у сплавах. Властивості зразка в цілому будуть змінюватися, коли два або більше металів об'єднуються для утворення сплаву. Важливо провести математичне моделювання електричного транспорту в металах і сплавах, особливо у рідкому стані. Лужні метали мають застосування в галузі ядерної енергетики. Літій, який має великий переріз поглинання, використовується як теплоносій в багатьох типах реакторів. Електронний струм може, в свою чергу, зумовлювати додатковий нагрів і, отже, підвищувати температуру самого теплоносія. Дана робота присвячена вивченню електричного транспорту в рідкому бінарному лужному сплаві на основі літію і натрію в різних співвідношеннях. За допомогою класичної теорії псевдопотенціалів досліджуються деякі важливі електричні транспортні властивості рідких бінарних сплавів $Li_{1-x}Na_x$. В статті вперше визначаються електричний опір, термоелектрична потужність та теплопровідність зазначеного сплаву з використанням універсального модельного потенціалу Файолхейза та ін. Різновиди функцій корекції локального поля (починаючи зі статичної діелектричної функції Хартрі (H) і закінчуючи обмінною та кореляційною функціями Хаббарда і Шама (HS), Тейлора (T), Вашішта і Сінві (VS), Фаріда та ін. (F), Ічімару і Уцумі (IU), Негі (N), у тому числі Саркара та ін. (S)) використовуються у даних розрахунках, що є загальновідомою практикою для подібних досліджень. Розраховані значення електричного опору досить добре узгоджуються з експериментальними даними.

Ключові слова: Електричний опір, Теорія псевдопотенціалів, Рідкі металеві сплави.