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COMPUTATION OF STRUCTURE AND ELECTRICAL RESISTIVITY OF LIQUID Na-Rb ALLOYS†

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The structure and electrical resistivity of $Na_{1-x}Rb_x$ binary alloys (where x = 0, 0.1, 0.2,…,1) are computed using Percus-Yevick (PY) equation, hard-sphere model and Faber-Ziman formula respectively. The partial structure factors and total structure factor are computed using hard-sphere model for $Na_{1-x}Rb_x$. In the calculation of resistivity using Faber-Ziman formula, we have employed Ashcroft empty-core pseudo-potential and Hartree dielectric screening. Calculated values of resistivity are compared with the experimental results and other theoretical values reported in literature. It is found that the electrical resistivity calculated using Faber-Ziman formula for binary alloy $Na_{1-x}Rb_x$ is in good agreement with the values reported experimentally.
Keywords: Structure factor, electrical resistivity, pseudo-potential, dielectric screening, liquid metal
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The study of structural and electron transport properties of liquid metals have attracted many researchers [1-2]. The studies related to liquid structure have been a concern for condensed matter physics and material science. The knowledge of the structural information and electron transport properties of liquid alloys are essential for understanding the alloys. Recently, the applicability of alkali-liquid metal alloys (such as Na-Rb, Na-K) in developing futuristic electrochemical devices makes it inevitable to study the electronic and chemical properties of such alloys [3-7]. The electrical resistivity of liquid binary alkali alloys has been computed theoretically by pairing Faber-Ziman formula [8] with a suitable pseudo-potential [9-10]. Islam et.al [9] has computed the electrical resistivity of $Na_{1-x}Rb_x$ binary alloys using Faber-Ziman formula employing Bretonnet and Silbert (BS) pseudo-potential [10] with two different local field corrections viz. Ichimaru-Utsumi (IU) and Vashishta-Singhwi (VS). It is important that a suitable potential associated with electron-ion interaction is chosen for the computation of the electrical resistivity as the choice of electron-ion pair potential plays a crucial role in the study of electrical resistivity.

In this paper, we compute the partial structure factors of $Na_{1-x}Rb_x$ binary alloys (where x =0, 0.1, 0.2,…, 1) employing the solution of Percus-Yevick (PY) equation for a multi-component hard-sphere model given by Hoshino [11] and the electrical resistivity of $Na_{1-x}Rb_x$ binary alloy is computed using the method given by Faber-Ziman [8]. In the computation of electrical resistivity, we employ Ashcroft empty-core pseudo-potential [12] and the dielectric screening function due to Hartree [13-14]. The results obtained are compared with experimental results available in literature.

THEORY

Resistivity

The electrical resistivity of a liquid metal binary alloy is given by Faber and Ziman [8] as

$$\rho = \frac{3\pi m^2 \Omega_o}{4Ze^2\hbar^3 k_f^6}\int_0^{2k_f}\{c_1 S_{11}(q)V_1(q)^2 + c_2 S_{22}(q)V_2(q)^2 + 2\sqrt{c_1 c_2}S_{12}(q)V_1(q)V_2(q)\}\, q^3 dq. \quad (1)$$

Here Z is the valence of the liquid alloy and$Z = c_1Z_1 + c_2Z_2$, where c_1 and c_2 are the concentration of elements, $\Omega_o = c_1\Omega_1 + c_2\Omega_2$ is the atomic volume of the alloy system, $V(q)$ is the form factor, $S(q)$ is the structure factor and k_f is the Fermi wave vector define by $k_f = \left(\frac{3\pi^2 Z}{\Omega_o}\right)$.

For the computation of electrical resistivity, we have considered Ashcroft's empty core potential [12] given by

$$V(r) = \begin{cases} 0, & r \le R_c \\ -\frac{Ze^2}{r}, & r > R_c \end{cases}, \quad (2)$$

where R_c is the core radius. The values of R_C for the constituent elements Na and Rb is taken from the values given in [12]. The form factor with dielectric screening effect is given by

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$$w(q) = \frac{w_b(q)}{\varepsilon(q)} = -\frac{4\pi Z e^2}{q^2 \epsilon(q) \Omega_0} \cos qr_c \tag{3}$$

where $w(0) = -\frac{2}{3}E_f$.

Following Hartree's theory of dielectric screening, the dielectric screening function $\varepsilon(q)$ is given as [13]

$$\varepsilon(q) = 1 + \frac{4\pi e^2}{q^2} D(E_f) \left[\frac{1}{2} + \frac{4k_f^2 - q^2}{8qk_f} ln \left|\frac{2k_f + q}{2k_f - q}\right|\right], \tag{4}$$

where $D(E_f) = 3n/2E_f$ represents the density of states at the Fermi energy E_f, n is the number density.

Structure factor

Computation of partial structure factors is a crucial step in calculating the electrical resistivity of an alloy. The partial structure factor, following the definition of Ashcroft-Langreth [11, 12] is given by the following expression

$$S_{ij}(q) = \delta_{ij} + \sqrt{c_i c_j}(a_{ij}(q) - 1), \tag{5}$$

where, δ_{ij} is the Kronecker delta function, c_i and c_j are the concentration of components, and

$$a_{ij}(q) = 1 + n \int d\boldsymbol{r} \big(g_{ij}(r) - 1\big) \exp(i\boldsymbol{k} \cdot \boldsymbol{r}) .$$

Where n is the number density of the mixture and $g_{ij}(r)$ is the pair distribution function. For the detailed derivation and the analytical expressions of partial structure factors see Hoshino [11].

The total structure factor $S(q)$ of the alloy can be expresses by the weighted average of partial structure factors from equation (5) as

$$S(q) = \frac{c_1 b_1^2 S_{11}(q) + 2\sqrt{c_1 c_2} b_1 b_2 S_{12}(q) + c_2 b_2^2 S_{22}(q)}{c_1 b_1^2 + c_2 b_2^2} \quad , \tag{6}$$

where the weights b_1 and b_2 are the neutron scattering lengths of the component elements of the alloy [15] and c_1 and c_2 are the concentrations of the component elements of the alloy.

CALCULATIONS

For computing the structure factor of the binary alloys, we need to fix the hard-sphere diameters (σ_i), packing fraction (η_i), and the concentration of components of elements. The hard sphere diameters (σ_i) have been determined using the relation,

$$\sigma_i = \left(\frac{6\eta_i \Omega_i}{\pi}\right)^{1/3} \tag{7}$$

where the value of η_i (packing fractionof *i*th species) is adjusted at temperature 373K according to the following relationship [16].

$$\eta_i = A_i \exp(-B_i T). \tag{8}$$

The atomic volume Ω_i of the *i*th species is calculated using the experimental values of densities at the desired temperature using the formula [17]

$$b_i = b_o - (T - T_{mi}) \frac{db}{dT} \tag{9}$$

Where T_{mi} is the melting temperature and b_o is the density at melting point of the *i*th species. Here, the densities are adjusted to the temperature 373 K.

Accordingly, the calculated value of Ω_i, σ_i and the other input parameters at the desired temperature are listed in Table 1.

Table 1. Input parameters use in calculating the structure factor and electrical resistivity of $Na_{1-x}Rb_x$ binary alloy

Element	T (K)	Valence (Z)	Ω_0 (a.u.)	σ (a.u.)	R_c (a.u.)
Na	373	1	278.240	6.265	1.663 [12]
Rb	373	1	659.220	8.279	2.722 [12]

RESULTS AND DISCUSSIONS

The representative partial structure factors and total structure factor as per the Ashcroft-Langreth [12]and Hoshino [11] for $Na_{50}Rb_{50}$ binary alloy is shown in Figure 1(a) and Figure 1(b) respectively. Using the partial structure factors for different compositions, the electrical resistivity of $Na_{1-x}Rb_x$ binary alloy system is computed. The electrical resistivity of $Na_{1-x}Rb_x$ binary alloy calculated at 373K using the Faber-Ziman formula [8] given in equation 1 are shown in Figure 2 along with the available experimental data reported by Hennephof et al. [17]. As seen in Figure 2, the result of the resistivity for $Na_{1-x}Rb_x$ binary alloys reported in this paper are very close to the data reported in literature.

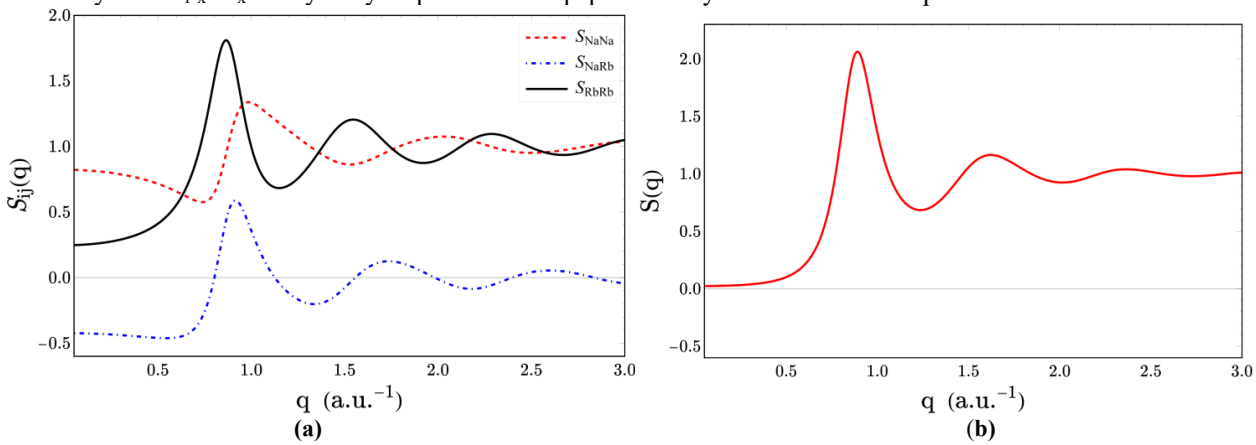

Figure 1. Representative partial structure factors $S_{ij}(q)$ and total structure factor $S(q)$ for $Na_{50}Rb_{50}$ binary alloy. (a) Partial structure factor of $Na_{50}Rb_{50}$, dashed, dot-dashed and solid lines represent Na-Na, Na-Rb and Rb-Rb respectively. (b) Total structure factor of $Na_{50}Rb_{50}$ binary alloy.

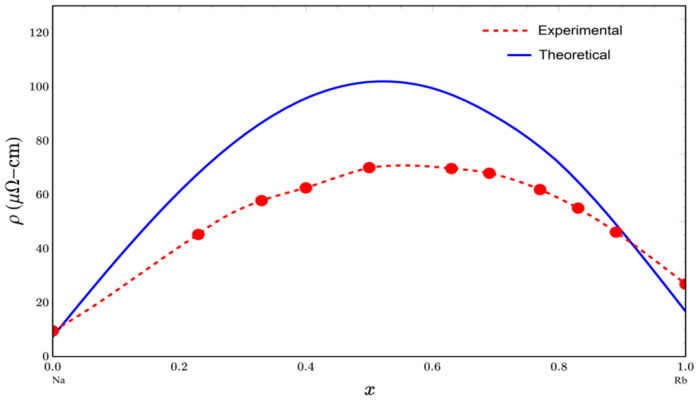

Figure 2. Resistivity of $Na_{1-x}Rb_x$ with concentration at 373K along with the experimental value [17].

We have used Ashcroft empty core pseudo-potential and Hartree dielectric screening function for computing resistivity of $Na_{1-x}Rb_x$ binary alloys. The results reported in this paper show better agreement with experimental data compared to previous theoretical study on resistivity of $Na_{1-x}Rb_x$ binary alloys as reported by Islam et.al [9] employing BS pseudo-potential along with Ichimaru-Utsumi (IU) and Vashishta-Singhwi (VS) dielectric field corrections.

CONCLUSIONS

We have computed the partial structure factors and total structure factor of $Na_{1-x}Rb_x$ binary alloys following the method prescribed by Ashcroft-Langreth [12]. The partial structures obtained for $Na_{1-x}Rb_x$ binary alloys were used for calculating electrical resistivity of $Na_{1-x}Rb_x$ binary alloys using Faber-Ziman formula [8]. In calculating the resistivity, we have employed Ashcroft empty core pseudo-potential along with Hartree dielectric screening function. The results obtained show good agreement with the experimental data available in literature. The use of Ashcroft empty core pseudo-potential along with Hartree dielectric screening for computing resistivity of $Na_{1-x}Rb_x$ binary alloys by Faber-Ziman formula shows good results. We are also working on the computation of the electrical resistivity of other alkali metal binary alloys using this approach.

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РОЗРАХУНОК СТРУКТУРИ ТА ЕЛЕКТРИЧНОГО ОПОРУ РІДКИХ СПЛАВІВ Na-Rb

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Структура та питомий електричний опір бінарних сплавів Na1-xRbx (де x = 0, 0,1, 0,2,…,1) розраховані за допомогою рівняння Перкуса-Євіка (PY), моделі твердої сфери та формули Фабера-Зімана відповідно. Часткові структурні коефіцієнти та загальний структурний коефіцієнт розраховані за допомогою моделі твердої сфери для Na1-xRbx. При розрахунку питомого опору за формулою Фабера-Зімана ми використали псевдопотенціал Ешкрофта з порожнім сердечником і діелектричне екранування Хартрі. Розраховані значення питомого опору порівнюються з результатами експерименту та іншими теоретичними значеннями, наведеними в літературі. Встановлено, що питомий електричний опір, розрахований за формулою Фабера-Зімана для бінарного сплаву Na1-xRbx, добре узгоджується з експериментальними значеннями.

Ключові слова: структурний фактор, питомий електричний опір, псевдопотенціал, діелектричний екран, рідкий метал.