A model potential and Ziman formulation is employed to study the temperature sensitiveness of electrical resistivity of liquid ternary alloys of Na-K-Rb. The calculated structure factors and form factors are employed for the numerical investigation of electrical resistivity for temperatures in the range 100-500°C. The binary combinations Na-K, Na-Rb show the Nordheim parabola for increasing temperatures, but there is an exception to K-Rb alloy system. The good agreement for electrical resistivity for pure liquid metals and their binary combination is achieved. The results of electrical resistivity for the ternary combination Na-K-Rb rise with temperatures.

Keywords: Pseudopotential, Electrical resistivity, Alloys, Liquid ternary alloys

IPC Code: G01L

1 Introduction

A number of researchers have reported the study on electrical resistivity of simple metals and their binary alloys. The interesting results emerging out from those works have motivated researchers to extend it for ternary systems. But the extensive investigation related to multi-component liquid metallic alloys of simple metals is still to be explored fully under Fiber-Ziman formulation and pseudopotential theory. It was also pointed out by Jin et al. that Ziman type theory can be applied successfully in the prediction of the electronic transport properties for simple binary alloy systems but a close examination of its applicability to multi-component systems is still needed. These all motivated us to consider further application of the pseudopotential theory and Ziman formulation to study electrical resistivity of alloys containing three different simple metallic constituents Na-K-Rb. The ternary systems of alkali Na-K-Rb are of our prime focus to calculate the temperature variation of electrical resistivity because alkalis Na, K and Rb are simple in electronic structure and of comparable size. The results of electrical resistivity on Na-K, Na-Rb and K-Rb are available in the literature, but data of electrical resistivity of Na-K-Rb are not available. So the present study would give a new set of data for future comparison on these ternary systems.

2 Theory

The calculations of electrical resistivity of Na-K-Rb have been performed for the ternary liquids at 100, 200, 300, 400 and 500°C for varied concentration range of (0.6,0.2,0.2), (0.4,0.2,0.4), (0.4,0.4,0.2), (0.2,0.2,0.6), (0.2,0.4,0.4) and (0.2,0.6,0.2). Our well established form factor is employed to explain inter atomic pair potential in the aforesaid liquids. The effective interaction pair potential for the ternary alloy system A-B-C is computed by

\[ V(r) = C_A^2 V_{AA}(r) + C_B^2 V_{BB}(r) + C_C^2 V_{CC}(r) + 2C_A C_B V_{AB}(r) + 2C_B C_C V_{BC}(r) + 2C_A C_C V_{AC}(r) \] … (1)

where

\[ V_{ij}(r) = Z_i Z_j r^{-1} \left( 1 - \frac{\pi}{\alpha} \int_0^\infty dq \left[ F_{ij}(q) + F_{ji}(q) \right] q^{-1} \sin(qr) \right) \] … (2)

Here, \( i = j \) gives us the pair potentials of A-A, B-B, C-C combinations while \( i \neq j \) will in turn the pair potential of mixed binaries like A-B, B-C and A-C. \( C_A, C_B \) and \( C_C \) denote the concentration of pure metals A, B and C, respectively, with the condition that \( C_A + C_B + C_C = 1 \). The energy wave number characteristics appearing in Eq. (2) is written as.
\[ F(q) = \frac{-\Omega_0 q^2}{16\pi} \left| W_q(q) \right| \left[ \frac{\epsilon(q)-1}{1+\epsilon(q)-1} \right] \left[ 1 - f(q) \right] \]  

... (3)

where, \( W_q(q) \) is the effective bare ion potential, \( \epsilon(q) \) be the Hartree dielectric response function and \( f(q) \) be the Taylor’s local field correlation function to introduce the exchange and correlation effects. The bare-ion model potential used in the present case is (in \( r \) – space):

\[ V(r) = -\frac{Ze^2}{r_c^2} \left[ 2 - \exp \left( \frac{1-r}{r_c} \right) \right] r^2; \quad r \leq r_c \]  

\[ = -\frac{Ze^2}{r}; \quad r \geq r_c \]  

... (4)

Here \( Z, e, r_c \) and \( \Omega_0 \) are the effective valence, electronic charge, parameter of the potential and effective atomic volume of the system, respectively.

The calculations of pair potentials of Na-K-Rb has been performed for the ternary liquids at 100, 200, 300, 400 and 500°C and at varied concentration range of Na-K-Rb viz; (0.6,0.2,0.2), (0.4,0.2,0.4), (0.4,0.4,0.2), (0.2,0.2,0.6), (0.2,0.4,0.4) and (0.2,0.6,0.2). The generated pair potentials are shown in Figure 1.

From the computed pair potentials of the ternary systems, we found that with the increase in concentration of heavy metals, the depth of the pair potential shifts towards higher value of \( r \) and is maximum for Na\(_{0.2}\)K\(_{0.2}\)Rb\(_{0.6}\) system at all the temperatures considered in the present study. The numerical calculation of the pair potentials is necessary for computing the hard-sphere diameter \( \sigma \), which can be determined using a relation

\[ V(\sigma) = V(r)^{\min} + \frac{3}{2} k_BT \]  

... (5)

where \( V(r)^{\min} \) is the depth of the first minimum in the pair potential, \( k_B \) the Boltzmann constant and \( T \) is the temperature.

Fig. 1—Pair potentials of liquid Na-K-Rb at \( T = 100, 200, 300, 400 \) and 500° C
Table 1 presents the numerical constants used in the present computation. The $\eta$ is calculated from Eq. (5), which then used to compute $\eta$. The $k_i$ and $Q_i$ are taken from the metallic data\textsuperscript{5-8,12-14}. The parameter of the potential $r_c$ is determined by satisfying $q = q_0$\textsuperscript{12-14} condition.

The electrical resistivity for ternary alloy system is computed using the formula\textsuperscript{11}

$$\rho = \left\{ \frac{3 \pi Q_0}{4k_F} \right\}^{2r_c} \int dq q^2 \left( C_1 a_1(q) W_1(q) \right) + C_2 a_2(q) W_2(q) + C_3 a_3(q) W_3(q) + 2(C_1 C_2)^2 a_{12}(q) W_2(q) W_1(q) + 2(C_1 C_3)^2 a_{13}(q) W_3(q) W_1(q) + 2(C_2 C_3)^2 a_{23}(q) W_3(q) W_2(q) \right\}$$

Herein $a_i(q)$ is the Ashcroft-Langreth partial-structure factor. $W_i(q)$ is the screened form factor and is calculated with exchange-correlation effects included for the i-type ion in a ternary alloy with different concentration.

The computed values of the electrical resistivities for Na-K-Rb liquids at different temperatures are summarized in Table 2.

Table 1—Input parameters used in the present study at $T = 200^\circ$C

<table>
<thead>
<tr>
<th>Metallic glasses</th>
<th>Z</th>
<th>$k_p$ (a.u.)</th>
<th>$Q_0$ (a.u.)</th>
<th>$\eta$ (a.u.)</th>
<th>$r_c$ (a.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>1</td>
<td>0.4315</td>
<td>416.44</td>
<td>0.4225</td>
<td>2.2771</td>
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<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>1</td>
<td>0.4080</td>
<td>494.82</td>
<td>0.4143</td>
<td>2.4096</td>
</tr>
<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>1</td>
<td>0.4131</td>
<td>469.30</td>
<td>0.4147</td>
<td>2.4164</td>
</tr>
<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
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<td>0.3845</td>
<td>573.20</td>
<td>0.4061</td>
<td>2.5421</td>
</tr>
<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>1</td>
<td>0.3895</td>
<td>547.68</td>
<td>0.4065</td>
<td>2.5490</td>
</tr>
<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>1</td>
<td>0.3946</td>
<td>522.16</td>
<td>0.4069</td>
<td>2.5558</td>
</tr>
</tbody>
</table>

Table 2—Electrical resistivity (in $\mu\Omega$.cm) for Na-K-Rb ternary liquid alloys at $T = 100$, 200, 300, 400 and 500$^\circ$C

<table>
<thead>
<tr>
<th>Liquid alloy</th>
<th>Electrical resistivity $\rho$ (in $\mu\Omega$.cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>100$^\circ$C</td>
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<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>57.26</td>
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<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>53.82</td>
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<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>47.39</td>
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<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>43.28</td>
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<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>41.60</td>
</tr>
<tr>
<td>Na$_0$K$_0$Rb$_0$</td>
<td>42.97</td>
</tr>
</tbody>
</table>

3 Results

The value of electrical resistivity increases from Rb-rich alloys to Na-rich alloys and is having maximum value for Na$_0$K$_0$Rb$_0$. This tendency is not linear with respect to the concentration. The minimum value for electrical resistivity is found for Na$_0$K$_0$Rb$_0$ at temperatures 100 and 200$^\circ$C. For $T = 300$, 400 and 500$^\circ$C, the electrical resistivity of Na$_0$K$_0$Rb$_0$ is found to be minimum. It indicates that, with the increase in temperature, the electrical resistivity decreases with the increase in concentration of heavier metals K and Rb for Na-K-Rb ternaries. The calculated values for ternary alloy signify the applicability of our model potential which observes the gradual changes of electrical resistivity with respect to temperature, but a nonlinear tendency with respect to the change in the concentration.

The good agreement for electrical resistivity for pure liquid metals and their binary combination was achieved by the present model potential\textsuperscript{16}. The experimental and other theoretical results of electrical resistivity on Na-K, Na-Rb and K-Rb are available in the literature\textsuperscript{5-7}, but the data on electrical resistivity of Na-K-Rb are not available. Hence in the absence of such results, the present study would give a new set of data for future comparison on these ternary systems.

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References


