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Free Energy of Mixing, Heat of Mixing and Viscosity of Na-K Liquid Alloy at Different Temperatures

H. K. Limbu[1, *], G. P. Adhikari[1], K. K. Mishra[2], K. Neupane[3] and I. S. Jha[2]
[1]Department of Physics, Tri-Chandra Multiple Campus, T. U., Ghantaghar, Kathmandu, Nepal
[2]Department of Physics, Mahendra Morang Aadarsh Multiple Campus, T. U., Biratnagar, Nepal
[3]Central Department of Physics, Tribhuvan University, Kathmandu, Nepal
[*]Corresponding Email: sewarohem@yahoo.com

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ABSTRACT

The Free energy of mixing, Heat of mixing and Viscosity of Na-K alloy are investigated theoretically at different temperatures using the Regular solution model. The interaction energy is temperature dependent. The theoretical values of interchange energy at different temperatures are obtained by best fit parameter approximation with the help of experimental values at 384K. The properties have been studied with the help of computed theoretical interchange energy at different temperatures using interchange energy and temperature relation. A comparison of theoretical and experimental values at 384K shows that they are in good agreement and using this basis we have computed the values at different temperatures.

Keywords: Regular solution model, Interaction energy, Free energy of mixing, Heat of mixing, Viscosity, Different temperatures.

INTRODUCTION

Sodium and Potassium are highly reactive and electropositive metals. Na-K is manufactured industrially in a reactive distillation [1]. The alloy is stored under hydrocarbons like hexane or inert gas like dry nitrogen or argon as it may ignite easily on exposure to air and highly reactive with water [2]. It is low melting eutectic alloy [3]. It has high surface tension, specific heat capacity and thermal conductivity. It can be used as an ideal heat transfer fluid in a storage system and as a coolant in experimental fast neutron nucleus reactors [4].

The regular solution model [5] has been used in this work. We have studied free energy of mixing (G_M), heat of mixing (H_M) and viscosity (η) at temperatures 384K, 400K, 450K, 500K, 550K, 650K, 750K, and 850K. And, viscosity of the alloy is calculated with the help of the Moelwyn-Hughes equation [6-7]. Many researchers have been working on several models to explain the mixing behavior of binary liquid alloys [8-13].

FORMALISM

Regular alloy constituent atoms A and B. The binary liquid alloy A-B of the homogenous solution consists of $C_{A\,(A=Na)}$ ($\equiv$c) mole of A and $C_{B(B=K)}$ {$\equiv$(1-c)} mole of B respectively.

The free energy of mixing (G_M) of binary liquid alloy is

$$G_M = G_M^{id} + G_M^{XS} \quad \text{.....(1)}$$

Where, excess free energy of mixing (G_M^{XS}) and ideal free energy of mixing (G_M^{id}) are given by

$$G_M^{XS} = \omega c_A c_B \quad \text{.....(2)}$$

and

$$G_M^{id} = RT\,[clnc + (1-c)ln\,(1-c)] \quad \text{.....(3)}$$

From equations (1), (2), and (3), we get

$$G_M = RT\,[c\,ln\,c + (1-c)ln(1-c)] + c(1-c).\omega \quad (4)$$

Where, T stands for temperature, ω is interaction energy and R is the molar gas constant.

The entropy of mixing (S_M) is given by

$$S_M = -\frac{\partial G_M}{\partial T} \quad \text{..... (5)}$$

From equation (4), we get

$$\frac{S_M}{R} = -[c\ ln\ c + (1-c)ln(1-c)] - c(1-c).\frac{1}{R}\frac{\partial \omega}{\partial T} \quad (6)$$

The importance of ω as temperature dependence has been studied by Bhatia et al. [14], Shrestha et al. [15], Alblas et al. [16]. The interchange energy (ω) is temperature dependent.

The relation between the heat of mixing (H_M), entropy of mixing (S_M), and free energy of mixing (G_M) is expressed as

$$\frac{H_M}{RT} = \frac{S_M}{R} + \frac{G_M}{RT} \quad \text{.....(7)}$$

Using equation (4), (6), and (7), we get

$$\frac{H_M}{RT} = c(1-c).\frac{\omega}{RT} - c(1-c)\frac{1}{R}.\frac{\partial \omega}{\partial T} \quad \text{.....(8)}$$

We have used the Moelwyn-Hughes equation to analyze the viscosity of Na-K liquid alloy which is given as

$$\eta = (c_1\eta_1 + c_2\eta_2)(1 - c_1c_2.\frac{H_M}{RT}) \quad \text{..... (9)}$$

Where, η_k (k = 1, 2) is the viscosity of pure component K and can be calculated from Arrhenius type equation [17] as

$$\eta_K = \eta_{OK} \exp\left[\frac{E_n}{RT}\right] \quad \text{..... (10)}$$

Where, η_{OK} is constant (in the unit of viscosity) and E_n is the energy of activation of viscous flow for pure metal (in the unit of energy per mole).

Order energy parameter at different temperatures

The values of free energy of mixing (G_M) of the alloy at different temperatures are computed from equation (4) using the values of order energy parameter (ω) at different temperatures from the relation [18, 19]

$$\omega(T) = A + BT \quad \text{.....(11)}$$

Where, A and *B* are coefficient constants.

RESULT AND DISCUSSION

The values of A and B is calculated using the values of ω/RT and $\frac{1}{R}\frac{\partial \omega}{\partial T}$ at temperature 384k of the alloy Na-K in equation (11). The best-fit parameters i.e., ω/RT = 0.961 and $\frac{1}{R}\frac{\partial \omega}{\partial T} = 0.041$ at temperature 384K by the method of best-fit approximation with the experimental values of the alloy from Hultgren et.al. 1973 [20] using equations (4) and (6). The theoretical values of interchange energy (ω) at different temperatures are calculated using equation (11) which is presented in the table 1.

Table 1: Interaction energy parameter (ω) at different temperatures

Temperature (T)	Order energy parameter (ω/RT)
384K	0.9610
400K	0.8535
450K	0.7632
500K	0.6910
550K	0.6319
650K	0.5410
750K	0.4743
850K	0.4233

Interaction energy is found to be positive at all temperatures which indicates homo-coordination [20]. Using these values of the interaction energy (ω), we have computed free energy of mixing (G_M), entropy of mixing (S_M), heat of mixing (H_M), and viscosity (η) at different temperatures (T) with the help of regular solution model. The values of entropy of mixing (S_M) changes ignorable or are almost same at different temperatures (T).

Free energy of mixing

The values of free energy of mixing (G_M) of the alloy at temperatures 400K, 450K, 500K, 550K, 650K, 750K, and 850K have been calculated using the values of ω(T) in equation (4) over the entire range of concentration. The free energy of mixing (G_M) of Na-K liquid alloy at different temperatures of study in the concentration range C_{Na} = 0.1 to 0.9 is shown in figure (1).

The theoretical and experimental values [21] of G_M/RT of the alloy are in good agreement at 384K. The values of free energy of mixing are found to be negative which shows weekly interacting nature. At all temperatures of investigations, the minimum value is at C_{Na}=0.5 which indicates the symmetry in

free energy of mixing. As the temperature of the alloy increases, the values of G_M/RT decreases and vice-versa.

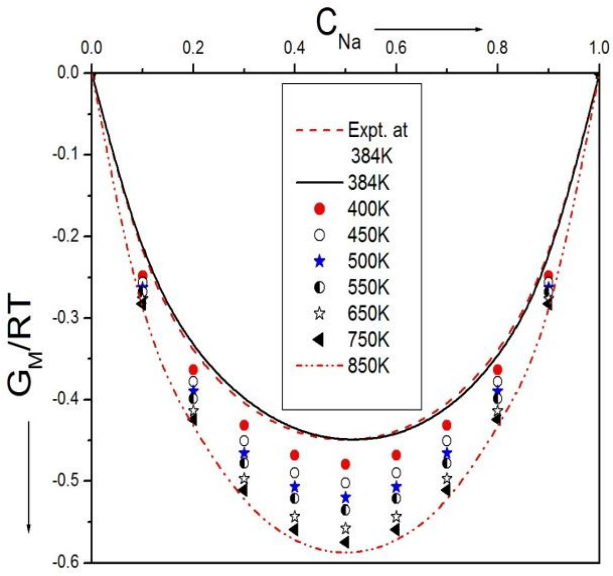

Fig.1: Graph for (G_M/RT) Versus the concentration of C_{Na} of Na-K liquid alloy at temperatures 384K, 400K, 450K, 500K, 550K, 650K, 750K, and 850K.

Heat of mixing (H_M)

The heat of mixing (H_M) for the alloy is calculated using equation (8) with the help of theoretical values of order energy parameter which is shown in figure 2.

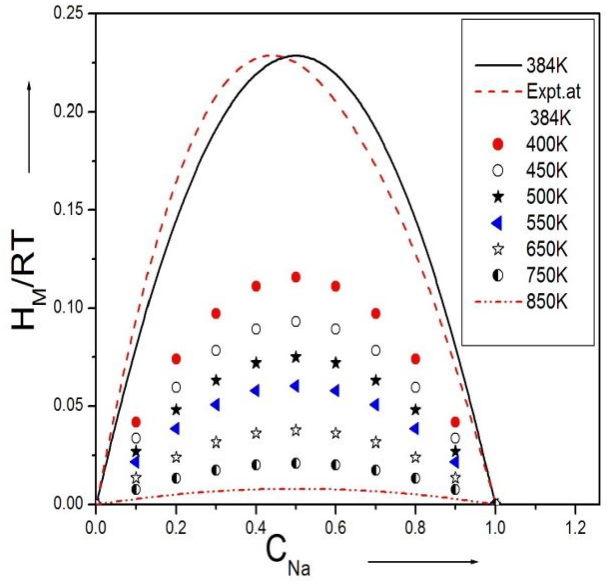

Fig.2: Graph for H_M/RT versus the concentration of C_{Na} of Na-K liquid alloy at temperatures 384K, 400K, 450k, 500K, 550K, 650K, 750K, and 850K.

The theoretical and experimental values of H_M/RT are in good agreement at 384K. The values of H_M/RT are positive in the entire concentration range at all temperatures and decrease with an increase in temperature from 384K to 850K. The values of H_M/RT are maximum at C_{Na}=0.5. Thus, the symmetry in heat of mixing is well explained.

Viscosity

The Viscosity of the alloy is calculated using equations (9) and (10). The viscosities of pure components Na and K at all temperatures(T) are computed using equation (10) with the help of constants η_{ok} and E for the metals [17] which is used to find the viscosity of the alloy for corresponding temperatures using equation (9).

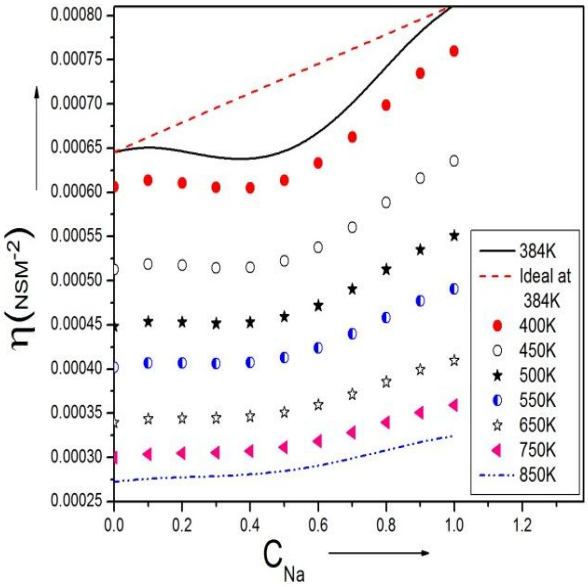

Fig. 3: Viscosity of Na-K liquid alloy at 384K, 400K, 440K, 500K, 550K, 650K, 750K, and 850K versus concentration of Na.

The viscosity of the pure component of Na atom is more than the viscosity of pure component K at all temperatures of study. The viscosity of the alloy is temperature dependent and decreases with the increase in temperature at each concentration range and minimum at 850K.

CONCLUSIONS

The free energy of mixing and heat of mixing show symmetric in nature at all temperatures of investigation. Viscosity decreases as the temperature of the study increases. Using temperature and interaction energy relation

different properties can be studied theoretically at different temperatures.

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