GLASS TRANSITION IN LIQUID BINARY ALLOYS

Deepika Bhandari,

Department of Physics, LBS Government College, Kotputli (Jaipur).

Romila Karnawat,

Department of Chemistry, Government PG College, SawaiMadhopur.

ABSTRACT

The liquidus temperature of two binary disordered Na-K and K-Cs systems has been calculated by extending Lindemann's melting criteria. The glass-forming ability has been computed in terms of an empirical parameter using the phase diagrams that were obtained. The tendency for forming glass is present in both binary systems.

Keywords: *Binary alloys, Phase diagram, Glass forming ability, Glasses.*

INTRODUCTION

The nature of liquid glass transition phenomena has long been a subject of interest in investigation in material science [1]. A thorough understanding of thermodynamics and phase diagrams is crucial to investigate liquid glass transition processes in liquid alloys. To study the theory of melting, several theoretical models have been designed [2]. Due to its simplicity and applicability to a wide variety of substances, Lindemann's melting criteria has a distinct position among these other models. [3, 4].

Moreover, the practical utility of metallic glasses makes glass-forming ability even more crucial. The glass-forming ability of two simple binary systems, Na-K and K-Cs, has been investigated utilizing their respective liquidus curves in light of the aforementioned information.

THEORY

According to Lindemann's criterion of melting, when a crystal melts, the mean square amplitude of its atomic vibrations exceeds some fixed part of the nearest neighbor distance (X_m), known as Lindemann's Constant. This constant depends on symmetry [5]. Further, for the crystals, having the same symmetry [5], the mean square deviation or uncertainty in the position at their respective melting points shall constitute the same part of their nearest neighbor distance. The generalized Lindemann's criterion of melting gives the melting temperature of an alloy [6]. The melting temperature of a binary alloy A_xB_{1-x} can be given as:

$$T_m = \left[\frac{Mk_B\theta_D^2}{9h^2}\right] a^2 X_m^2 \left(1 - \frac{X_p^2}{X_m^2}\right) \quad .....(1)$$

Where, X_m^2 = 0.0218 is the Lindemann constant [7], M is the average atomic mass, is the Debye temperature and it is expressed as

$\theta_D^{-2} = x\theta_{D_A}^{-2} + (1-x)\theta_{D_B}^{-2}$, a is the nearest neighbor distance. The mean square size dispersion X_P^2 can be expressed in terms of the hard-sphere diameter of constituents hard sphere diameters σ_A and σ_B as [8]:

$$X_p^2 = a^{-2}X(1-X)(\sigma_A - \sigma_B)^2$$

The liquidus curves can be drawn by melting temperature T_m in the complete range of

composition. The glass forming ability (GFA) parameter [9] gives information about the particular composition at which a metallic system is likely to form a glass by the melt quenching technique. This parameter can be expressed in terms of an empirical parameter:

$$\Delta T^{*} = \frac{\left(T_{liq}^{mix} - T_{liq}\right)}{T_{liq}^{mix}} \quad \ldots\ldots(2)$$

Where, $T_{liq}^{mix} = xT_{liq}^{A} - (1-x)T_{liq}^{B}$ in which T_{m}^{A} and T_{m}^{B} are the melting points of the constituents A and B in a simple binary alloy A_xB_{1-x} in their normal isolated state. The GFA parameter characterizes the fractional departure of liquidus temperature T_{liq} from that of the simple rule of mixture liquidus temperature T_{liq}^{mix}. In research [10], it was observed that the binary and ternary alloys which have $\Delta T^{*} > 0.2$, were readily glass forming by melt quenching with only 8 exceptions to the rule. This provides a reasonably reliable indication that the values $\Delta T^{*} > 0.2$, a metallic system is likely to form glass by melt quenching technique, provided its liquidus temperatures are known.

RESULTS AND DISCUSSION

The melting temperature for binary alloys namely Na-K and K-Cs were determined using Eq. 1 for the entire composition. Based on observations, the following conclusions have been drawn:

NA-K System

The phase diagram of binary alloys is computed using Eq.1. The hard sphere diameter of liquid metal components has been taken from the work of Hafner[11] and Debye temperature from that of Faber [12]. The glass-forming ability parameter ΔT^{*} is calculated knowing the melting temperature of the system in the entire range of composition using Eq.2. Both the phase diagram and GFA parameter are shown in Fig,1.

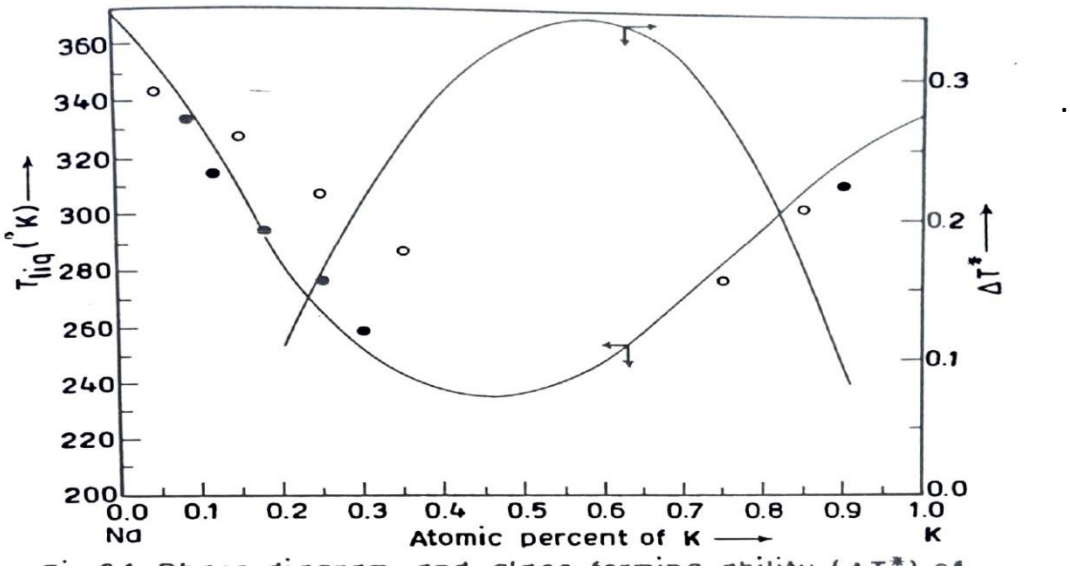

Fig.1: Phase Diagram and Glass Forming Ability of Na-K alloy: _____ Present computed results, o,o,o,o experimental results, ... points from ideal solution

The experimental results are also displayed for comparison. It can be seen from Fig that theoretical results match qualitatively fairly well with the experimental results. The GFA parameter comes out to be 0.33 at the composition $Na_{0.32}K_{0.68}$ predicting it to be glass forming. This prediction matches with that of Bhatia and March [9[.

K-Cs System

Similar to the Na-K system, the phase diagram of K-Cs alloy has been determined using Eq.1. The computed phase diagram is shown in Fig.2. Since there is negligible difference in electronegativity values between K and Cs, the charge transfer effect is not considered and values of hard sphere diameter have been taken the same for the entire range of composition.

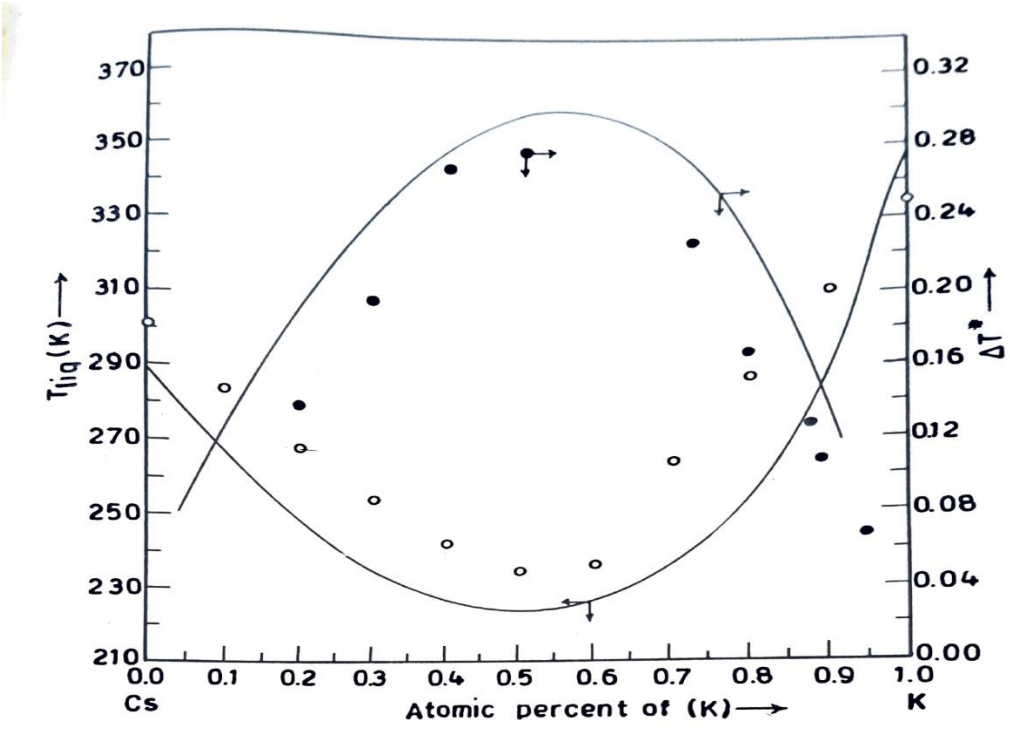

Fig.2: Phase Diagram and Glass Forming Ability of K-Cs alloy: _____ Present computed results, o,o,o,o experimental results, ... points of $S_{CC}(0)$ from work [14].

The present phase diagram matches the reported experimental results [13]. The GFA parameter is also computed through Eq. 2 using the calculated liquidus temperature at all compositions. The GFA parameter and the liquidus temperature curve are also displayed in Fig.2. For K-Cs alloys its value comes out to 0.299(~0.3) at equiatomic composition predicting it to be glass forming.

CONCLUSION

From the above results, it can be concluded that the Lindemann criterion of melting gives quite satisfactory results in determining the phase diagram and glass-forming ability of a binary disordered system. The above results suggest both binary systems have glass forming tendency.

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