Structural Dependence of Compound Forming Liquid Binary Alloys

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Abstract- Most of experimental evidences clearly demonstrates that the anomalous behaviour for a large number of liquid alloys occur at or near the stoichiometric compositions where stable intermetallic compound exist in the solid phase. It is therefore, natural to propose that the chemical complexes, associations clusters or pseudopotential exist in the liquid phase near the melting temperature. An appropriate estimation of the stoichiometry of complexes in the liquid alloy is usually model by an analysis of anomalous composition dependence of the physical properties and also from the phase diagram. The complex forming model successfully explains the thermodynamic properties of number of compound forming alloys.

Keywords- Intermetallic compound, chemical complexes, pseudomolecular

1 INDRODUCTIONS

The thermodynamic properties like free energy of mixing G_M, Heat of mixing H_M and many other electronic properties are symmetric about the equiatomic Composition of many liquid binary alloys. The liquidus lines for these system are complicated and are usually S- shaped. These alloys have the characteristics that in the solid phase. They form compound at one or more stoichiometric compositions.

2 COMPLEX FOROMING MODEL

The asymmetry of the properties of mixing for liquid binary alloys could be explained on the assumption of chemical complexes.

$$\alpha A + \beta B = A\alpha B\beta$$

Where α and β are small integers, A and B are the constituent species.

Thus a binary alloy in the liquid phase can be considered as a ternary mixture of left over A, B atoms and the chemical complexes $A\alpha B\beta$ all in chemical equilibrium.

Let a binary liquid alloy contains in all c gm atoms of A and (1-c) gm atoms of B. On considering the existence of only on type of chemical complexes. the binary alloys can be assumed to be consisted of n_1 gm atom of A and n_2 gm of atom of B and n_3 gm atoms of the complexes $A\alpha B\beta$.

$$N_1 = c - \alpha n_3$$

$$N_2 = 1 - c - \beta n_3$$

And $$n = n_1 + n_2 + n_3$$
$$= 1 - (\alpha + \beta - 1) n_3$$

Let G_i denotes the chemical potentials per atom of the species in its pure stats, then the free energy of mixing G_M of the binary liquid alloy may be expressed as

$$G_M = G - cG_i - (1-c) G_2$$
$$= - n_3 g + G'$$

Where G is the total Gibb's free energy of the mixture and

$$G = {}_{\alpha} G_1 + \beta G_2 - G_3$$

The simplest expression for G' can be obtained assuming that ternary mixture forms an ideal solution so G' may be expressed as

$$G' = G - \sum_{i=1}^{3} n_i G_i$$

Using Euler's theorem for identify between an extensive variables

$$G' = RT \sum_{i=1}^{3} n_i \ln \left(\frac{n_i}{n}\right)$$

Therefore , the expression for the free energy of mixing

$$G_M = - n_3 G + RT \sum_{i=1}^{3} n_i \ln \left(\frac{n_i}{n}\right) + \sum\sum_{i<j} \frac{n_i n_j}{n} w_{ij}$$

In case of conformal solution model $W_{ij} \to 0$ and $n_3 \to 0$, then

$$G_M = RT\,[clnc + (1-c)\ln(1-c)]$$

The free energy of mixing has been calculated using above expression.

3 RESULTS AND DISCUSSION

Free energy of mixing G_M/RT, as a function of concentration for a fixed value of equilibrium constant K= 4.54×10^{-5} and considering interaction energy $W_{ij}=0$ and for different values of α and β are marked.

For each of computed numerical values of k, the equilibrium constant, the values of G_M/RT computed and found that for a given set of α and β, the minimum G_M/RT occurs ot the same concentration Further its observe that a smaller K corresponds to minimum in G_M/RT the slop of G_M -c curves on either sides of minimum depends strongly on the values of K. The slop in more steep for lower values of K but become flatten as K increases.

4 EFFECT OF W_{ij} ON FREE ENERGY OF MIXING G_M

In order to see the impact of W_{ij}, interaction energies of constituent species on free energy of mixing, first of all positive values of W_{ij} on free energy of mixing of four different sets [$W_{ij}=0$; $W_{12}/RT = 10.0$; $W_{13}/RT = 0.0$; $W_{23}/RT = 10$, $W_{12}/RT = W_{23}/RT = 0$ and $W_{23}/RT = 10.0$, $W_{12}/RT = W_{13}/RT = 0$] have be taken and computed.

It has been observed that the position of minimum in G_M/RT not only depends upon the values of α and β but also depends on the values of W_{ij}. The values of W_{ij} as given above in set (a) and (b) almost yield identical G_M/RT. The sets (c) also yields the same values of G_M/RT upto $c < 0.5$ but differs considerably for $c \geq 0.5$ The fourth set of W_{ij} gives much smaller values of G_M/RT in the lower concentration region but becomes identical for light concentration.

The effect of negative values of W_{ij} on G_M is more appearance.

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