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THE ESTIMATION OF STRUCTURAL INHOMOGENEITIES IN MOLTEN ALLOYS BY MEANS OF RMC_METHOD

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INTRODUCTION

Most of structural studies of metallic alloys show the existence of inhomogeneous atomic arrangement in liquid state. This feature of structure is more pronounced at temperatures, which are close do liquidus curve. The appearance of anomalous point in temperature and concentration dependencies of structure parameters are commonly considered as evidence of inhomogeneities in liquid state. These parameters can be obtained from diffraction data and physical-chemical properties measurements.

Nevertheless the description of inhomogeneities of short range order by means of structure parameters analysis is restricted. Use of some models leads to a little progress but there is no powerful method for studing of inhomogeneities in melts.

Liquid metals also show the inhomogeneous structure. For example, liquid semimetals and semiconductors, whose structure factors can be considered as consisting the two kind structural units: close packed with metallic bonding and of less density with covalent one. [1] It was shown that fraction of second kind units decreases with temperature. In binary metallic systems, whose phase diagram exhibit the chemical compounds , the inhomogeneities of structure are caused by existence of chemically ordered units, which are diluted in matrix of basic metal. In many cases for description of inhomogeneities in binary melts the thermodynamic data are used. For this purpose the integral enthalpy of mixing is needed. Using this characteristic the fraction of chemically ordered atomic groups can be calculated. Such approach is known as a model of associates [2].

Similar model was used for interpratation of structure factors. This model is based on the assumption that scattered intensity is an additive sum of intensities for each kind atomic groups.

In this paper we propose to use the reverse Monte-Carlo (RMC) method for interpretation of X-ray diffraction data for liquid atomic alloys, whose structure is inhomogeneous. For investigation alloys of eutectic systems were chosen.

EXPERIMENT

X-ray diffraction studies were carried out with using of high temperature diffractometer, which allows us to obtain the structure factors of high accuracy. During the experiment the chamber of diffractometer was filled with pure helium in order to avoid the oxidation of sample.

Model structure factors were calculated by means of RMC method [4]. The agreement between calculated and experimental structure factors was the starting point for obtaining of atomic arrangement within some definite cell. This also allowed us to determine the partial structure factors and partial pair correlation functions, from which the partial structure parameters, such as distances and number of neighbors of each kind, were estimated .

RESULTS AND DISCUSSION

For the estimation of chemical ordering in molten alloys the Warren parameter is commonly used [3]. It determines by relation

$$\alpha_w = 1 - \frac{N_{21}}{c_1 N_2}$$

where c_1 – is atomic fraction of first component; N_{21} – number of neighbors of first kind atoms respectively to second one, N_2 – number of neighbors around the second kind atoms.

Concentration dependencies of this parameter for $Al_{1-x}Ni_x$ and $Sn_{1-x}Cu_x$ is presented in Fig.1.

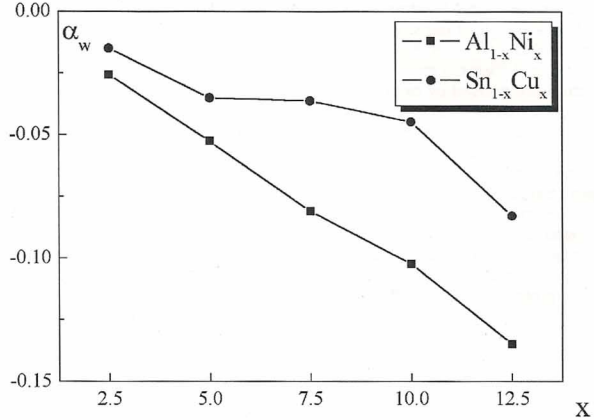

Figure 1. The ordering parameter for Al-Ni and Cu-Sn molten alloys.

These systems were studied early by means of X-ray diffraction method [5, 6]. As it can be seen there is a decrease of α_w value with concentration. It is in agreement with results on analysis of structure factors and pair correlation functions.

In the case of binary systems, which reveal the tendency to self-association, using of this parameter is no useful. Such tendency is observed in binary alloys, whose phase diagrams exhibit the miscibility gap or eutectic point.

We propose to use the ratio of number of self-associated atoms to total number of atoms:

$$\alpha_{s.a.} = \frac{N_{22}}{N_2}.$$

This parameter is used in order to describe the distribution of diluted atoms in some solutions. Number of diluted atoms which are in self-associated state and total numbers of atoms in cubic cell, whose volume was equil from 2.7 to 10 nm^3 were calculated by RMC method. Results are presented in Fig.2.

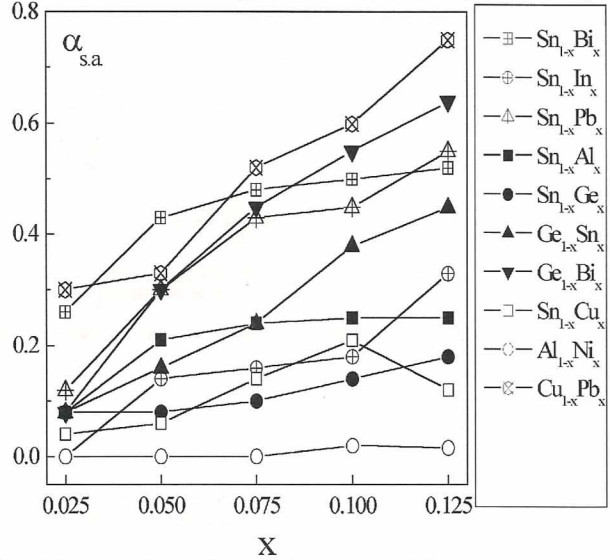

Figure 2. The parameter of self-association versus concentration.

It can be seen that this parameter increase with different rate. This increasing is most significant in $Cu_{1-x}Pb_x$ melts and shows the almost unchangeable value for $Al_{1-x}Ni_x$ molten alloys. Therefore the addition of lead atoms to copper can not be considered as formation of random atomic distribution. This is in agreement with data on analysis of structure factors and pair correlation functions. Besides, the phase diagram for Cu-Pb system exhibits the miscibility gap in liquid state.

For $Al_{1-x}Ni_x$ molten alloys a little tendency to self-association of diluted atoms is due to existence of heterocoordinated structure. For other tin-based solutions these is a different dependence of self-associated structural units fraction on concentration.

CONCLUSIONS

RMC method can be useful for estimation of the fraction of self-associated structural units in molten alloys. Existence of such units is the reason of inhomogeneous short range order even in melts, whose concentration lies within interval of diluted solutions.

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