Journal of Non-Crystalline Solids 364 (2013) 34–39

Contents lists available at SciVerse ScienceDirect

Journal of Non-Crystalline Solids

journal homepage: www.elsevier.com/ locate/ jnoncrysol

Formation of the short-range order in Al-based liquid alloys

O.S. Roik [a,*], V.P. Kazimirov [a], V.E. Sokolskii [a], S.M. Galushko [b]

[a] Chemical Department, National Taras Shevchenko University of Kyiv, Kyiv, Ukraine
[b] Pavlo Tychyna Uman State Pedagogical University, Uman, Ukraine

ARTICLE INFO

Article history:
Received 12 November 2012
Received in revised form 25 December 2012
Available online 1 February 2013

Keywords:
Al-based liquid alloys;
Chemical short-range order;
X-ray diffraction;
Reverse Monte-Carlo simulations;
Prepeak

ABSTRACT

The short-range order in binary and ternary liquid alloys of aluminum with 3d-transition metals (TM) was studied by the X-ray diffraction method and Reverse Monte Carlo simulations. The causes of the presence of the prepeak and asymmetric shape of the second peak on the experimental total structure factors were discussed. The effect of the transition metal atom type on the short-range order of Al-based liquid alloys was demonstrated.

1. Introduction

The most of known metallic structural materials can be obtained from the liquid state. So, the examination of regularities in the formation and evolution of the short-range order in the multicomponent metallic melts is an actual task of studies in the field of the modern materials engineering. Crystalline, quasicrystalline and amorphous phases can be obtained from the liquid aluminum based alloys depending on the composition and the alloy cooling rates, which have been used [1]. Therefore, different aluminum based alloys, which being in the equilibrium state and in the undercooled state, were studied by using neutron and X-ray diffractions [2–5]. It should be noted, that the study of the short-range order (SRO) of such liquid alloys is important not only for obtaining new structural materials, but also for understanding the nature of the liquid state.

The interaction between the atoms of different types and atomic packing density are two factors that affect on the formation of the local atomic structure of metallic melts. A difference in the electronegativity of such atoms causes strong interatomic interactions and the chemical short-range order (CSRO) can be realized. Simultaneously, the high atomic packing density of the metallic melts can be realized by the formation of dense non-crystalline atomic clusters. These factors should be taking into account at the SRO analysis in the case of liquid alloys of aluminum with transition metals. For example, experimental structure factors (SF) of binary and ternary liquid alloys of aluminum with 3d-transition metals (TM) have an additional peak at low values of the diffraction vector so-called prepeak [6–8], whose appearance is attributed to the presence of the medium-range order [9]. The prepeak usually is caused by the CSRO, the latter reduces contacts between the TM atoms [7,10,11]. Another feature of the SF of liquid Al-TM^{I} and Al-TM^{I}–TM^{II} alloys is the asymmetric shape of the second peak that is usually associated with the icosahedral short-range order (ISRO). [7,12]. Despite substantial interest to the experimental study and modeling the structure of Al-based liquid alloys, the studies on the effect of the size and the chemical type of atoms on the formation of the SRO are still actual.

Diffraction studies of liquid binary Al–TM alloys indicate that parameters of the SRO depend on the TM type [8,13] and the alloy composition [6,11], which is clearly seen in the concentration range from a pure aluminum to the binary $Al_{80}TM_{20}$ alloys. Consequently, addition of various TM to the liquid Al-based alloys can specifically change the local atomic order, the latter open up new possibilities for obtaining new structural materials based on aluminum with preset characteristics.

In this work we report the results of X-ray diffraction and RMC simulation of the Al-based liquid alloys with approximately the same content of aluminum and analyze the local atomic structure of these liquid alloys. X-ray diffraction studies of the liquid $Al_{80}Mn_{12}Cu_8$ and $Al_{80}Mn_{14.7}Ni_{5.3}$ alloys were carried out at temperatures approximately 50 K higher than the liquidus temperatures. The RMC simulations of liquid $Al_{80}Co_{20}$, $Al_{82}Ni_{18}$, $Al_{86}Cu_{14}$, $Al_{80}Mn_{20}$, $Al_{80}Ni_{10}Co_{10}$, $Al_{81.6}Ni_{14.9}Fe_{3.5}$, $Al_{80}Mn_{14.7}Ni_{5.3}$, $Al_{80}Mn_{12}Cu_8$, and $Al_{86}Ni_8Ce_6$ alloys were carried out using the experimental X-ray diffraction data from our earlier studies [12,14–17]. Voronoi–Delaunay method was used to examine atomic ordering in the RMC-models of all liquid alloys. The change of the local atomic order in the liquid Al-based alloys, which is realized via the partial substitution of the one kind of TM atom by another TM atom, was analyzed in details.

* Corresponding author. Tel.: +380 44 239 34 17.
E-mail address: sasha78@univ.kiev.ua (O.S. Roik).

0022-3093/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.jnoncrysol.2012.12.040