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Structure of liquid Al–Cu–Co alloys near the quasicrystal-forming range

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ABSTRACT

A local short-to-intermediate range order in liquid $Al_{63.9}Cu_{19.4}Co_{16.7}$, $Al_{71}Cu_6Co_{23}$, and $Al_{60}Cu_{29}Co_{11}$ alloys was investigated by X-ray diffraction technique and the reverse Monte Carlo modeling. A prepeak at $Q \sim 17$ nm^{-1} originating from the unique bonding between the TM–TM pair (TM = Co, Cu) is observed in the structure factors of all investigated melts. The Voronoi–Delaunay analysis of RMC models indicates that a medium-range ordering of TM atoms in dense non-crystalline polytetrahedral clusters is associated with a chemical short-range order. The icosahedral short-range order is also closely related to the dense packing polytetrahedral clusters. A decrease of temperature leads to an enhancement of both chemical short-range order and icosahedral short-range order.

1. Introduction

The discovery of quasiperiodic structures with icosahedral symmetry [1] has activated interest in the study of the relationship between short-range order (SRO) in quasicrystal-forming melts and in the corresponding solid phases. A great number of the quasicrystal (QC) materials can be obtained from the Al-based melts [2], therefore the SRO of these melts has been widely investigated. With the increasing number of studies, some structure features have attracted more and more attention. One of these features is the icosahedral short-range order (ISRO), that is more pronounced for melts forming quasicrystalline phases. This increases with decreasing temperature (mainly for undercooled state of liquid alloys) [3]. The second one is the prepeak on the low-Q side of the first peak in the structure factors (SF) of the liquid Al-based alloys.

The ISRO prevails in undercooled metallic melts due to energetic reasons [4]. Since the ISRO is incompatible with the translational periodicity of crystalline solids, an energy barrier for crystal nucleation exists. It explains the significant undercooling of metallic liquids. Later this hypothesis was confirmed for pure liquid metals and alloys [5–9]. Significant ISRO in the liquid Al-based alloys has been reported in [8–11]. The increasing prominence (with undercooling) of a shoulder on the high-Q side of the second peak in the experimental structure factor was consistent with a significant amount of the ISRO. The relationship between the ISRO and the shoulder on the high-Q side of the second peak was proved by the simulation of $S(Q)$ at $Q > 45$ nm^{-1} [7,8]. The experimental $S(Q)$s of $Al_{65}Cu_{25}Co_{10}$, $Al_{13}Fe_4$, and $Al_{74}Co_{26}$ melts were simulated under the assumption that such clusters with fcc, hcp or ISRO exist in the melt. The shoulder of second maximum of the $S(Q)$ is best described under the assumption of ISRO existence. The prevalence of the ISRO in the liquid Al-based alloys was also confirmed by neutron scattering studies [10–12]. The ISRO has been accompanied by a chemical short-range order so that the first coordination shell of a transition metal atom mainly consists of Al atoms [8,11,12].

The presence of a prepeak in the structure factors of the liquid Al-based alloys was reported in [3,12–18]. The prepeak position is lower than the position of the $S(Q)$ main peak, which is generally associated with the SRO. Therefore, the prepeak correlates with the order longer than the nearest interatomic distances, i.e. a medium-range order (MRO). The structural origin of the prepeak in the $S(Q)$ of the metallic melts is still a subject of dispute. The prepeak in the SF curve of liquid Al–TM (TM = Fe, Ni, Cu) alloys was explained by the presence of atomic clusters, whose composition corresponds to the stoichiometry of the solid intermetallics [14–16]. The prepeak phenomenon for a liquid $Al_{80}Ni_{20}$alloy was attributed to the Ni–Ni pairs, which results from a superstructure caused by Al–Ni interactions [17]. The molecular dynamic (MD) simulations of the liquid Al–Ni binary alloys [13] showed a prepeak, mainly present structure factor $S_{NiNi}(Q)$ for the Al-rich compositions. Direct experimental information concerning the nature of the prepeak was obtained in three neutron scattering experiments with different scattering contrasts of the components. Holland-Moritz et al. [12] studied undercooled $Al_{13}(Co_x, Fe_{1-x})_4$ melts with different x by neutron diffraction. The Faber–Ziman structure factors $S_{AlAl}(Q)$, $S_{AlTM}(Q)$ and $S_{TMTM}(Q)$ (TM = Co, Fe) were obtained, the prepeak appeared in the $S_{TMTM}(Q)$ curve at low Q-values. We have previously reported that prepeak is observed in the $S_{TMTM}(Q)$ of the Al–Ni, Al–Co, and Al–Cu melts in the Al-rich region [19,20].

This paper reports the short-to-intermediate range order in liquid $Al_{71}Cu_6Co_{23}$, $Al_{63.9}Cu_{19.4}Co_{16.7}$, and $Al_{60}Cu_{29}Co_{11}$ alloys near the

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