Icosahedral Short-Range Order in Undercooled Metallic Melts

Holland-Moritz D.

DLR, Institut für Raumsimulation, D-51170 Köln, Germany (email: dirk.holland-moritz@dlr.de)

It was predicted already in 1952 by Frank [1] that an icosahedral short-range order should prevail in undercooled metallic melts because of energetic reasons. Lateron, this hypothesis has been supported by a large number of theoretical investigations. Direct experimental information on the short-range order in undercooled metallic liquids, however, became available quite recently.

In this work diffraction experiments on the short-range order of stable and deeply undercooled melts of the pure elements Ni, Co, Zr, Fe and Ti and of Al-based alloys forming quasicrystalline or polytetrahedral phases ($Al_{13}(Fe,Co)_4$, $Al_{60}Cu_{34}Fe_6$, $Al_{65}Cu_{25}Co_{10}$) are presented. The liquids were containerlessly processed und undercooled by use of the electromagnetic levitation technique, which was combined with the techniques of elastic neutron scattering and energy dispersive diffraction of synchrotron radiation in order to determine the structure factors of the liquids as a function of the temperature.

For all of the above mentioned metallic liquids the measured structure factors are well described if an icosahedral short-range order is assumed to prevail in the melt, independently on the structure of the corresponding solid phases. The icosahedral short-range order is observed even at temperatures above the melting temperature and becomes more pronounced in the metastable regime of an undercooled liquid.

For the $Al_{13}(Fe,Co)_4$ melts that form polytetrahedral phases partial structure factors were determined. These indicate that in addition to an icosahedral topological short-range order there exists a pronounced chemical order such that the first coordination shell around a transition metal atom consists preferentially of Al-atoms.

References

[1] F.C. Frank, Proc. R. Soc. London A **215**, 43 (1952).