ESRF	**Experiment title:** Short-range order in melts **of** quasicrystal-forming alloys	**Experiment number:** CH-289
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Report:

Metallic melts can be deeply undercooled below the melting temperature, provided that heterogeneous nucleation at container walls or impurity sites is suppressed by application of suitable techniques of containerless processing, such as electromagnetic levitation. Undercooled melts are in a metastable state. Frank [l] suggested already in 1952 that an icosahedral short-range order should prevail in undercooled melts because of energetic reasons. This assumption was supported by molecular dynamic computer simulations on Lenard-Jones liquids [2,3], which showed an increasing degree of icosahedral short-range order with increasing undercooling of the melt. Especially for melts forming quasicrystalline phases, a pronounced tendency to form an icosahedral short-range order is expected, since for these alloys also the solid phases are characterized by icosahedral short-range order.

From the experimental side only some indirect studies of the dependence of the structure of the solid on the maximum undercoolability [4] are reported that are in favour of the idea of an icosahedral short-range order. In order to obtain a better insight into the short-range order of undercooled quasicrystal-forming melts, liquid droplets of $Al_{72}Pd_{21}Mn_7$ and $Al_{65}Cu_{25}Co_{10}$ were investigated by EXAFS at different temperatures. The samples of 7mm in diameter were containerlessly processed within a **specially designed electromagnetic** levitation facility [5].

Figure 1 shows the EXAFS amplitude as a function of the k-vektor rneasured at the K-edge of Co for an $Al_{65}Cu_{25}Co_{10}$ sample at a temperature of 1300 K (dotted symbols). EXAFS oscillations are clearly visible up to k-values of about 8 $Å^{-1}$.

The spectrum was analyzed under the assumption that the Co atoms have an environment with icosahedral symmetry, which also implies a coordination number of Z=12. A good fit of the experimentally observed spectrum could only be obtained, if it was assumed that nearly all nearest neighbours of the central Co-atom are Al-atoms at a distance of $R_{Al} = 2.54$ Å. The resulting fit is also plotted in figure 1 (solid line), highlighting that the theoretical curve delivers an excellent description of the measured data.

The analysis of the spectrum indicates that in $Al_{65}Cu_{25}Co_{10}$ melts there exists a tendency that Co-atoms are preferentially surrounded by Al-atoms. This result is well in line with the assumption of an icosahedral short-range order in the melt. In a cluster with icosahedral symmety the distance between the central atoms and the atoms on the surface is about 5% smaller than the distance of two neighbouring surface atoms. Because of these geometric reasons it is favourable if a small central atom (Co) is surrounded by larger atoms (Al). A similar behaviour is also known to occur for solid Frank-Kasper phases that are characterized by icosahedral symmetry elements within a large unit cell. Further investigations on the short-range order in quasicrystal-forming melts are necessary.

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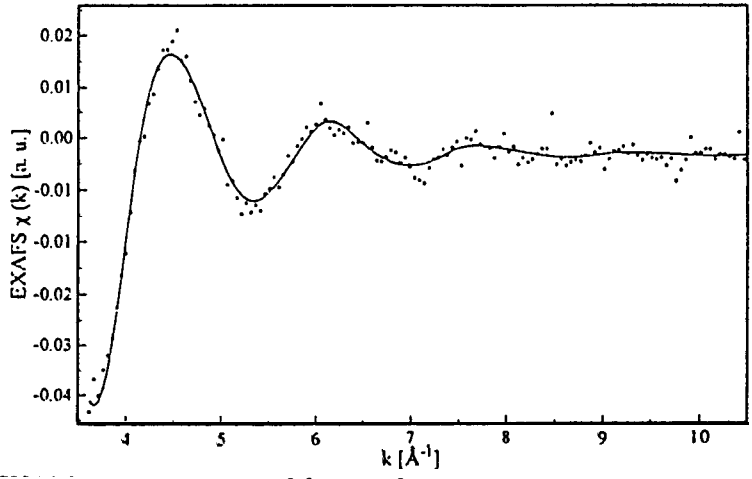

Fig. 1: EXAFS spectrum measured for a molten $Al_{65}Cu_{25}Co_{10}$ specimen at a temperature of T = 1300 K