ESRF	**Experiment title:** **X-ray diffraction on undercooled metallic melts**	**Experiment number**: HS-1286
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Report:

Already in 1952 Frank [1] has predicted that an icosahedral short-range order (SRO) would prevail in undercooled melts of atoms with sphere-like symmetry because of energetic reasons. Despite of some indirect studies on the SRO [2] which are in favour of Frank's idea and some first diffraction studies [3], little is known on the SRO of undercooled metallic melts. Therefore this experiment was intended to investigate the SRO of undercooled melts by X-ray diffraction. In order to deeply undercool metallic melts, heterogeneous nucleation has to be suppressed. This requires containerless processing of the melts under high purity conditions. For this an electromagnetic levitation facility was used, like in the experiments HS 178, HS 488 , HS 800, HS 802 which was combined with an energy dispersive X-ray diffractometer. However, due to difficulties which occured during the adjustment of the beamline, during the experiment HS 1286 only melts of Co, $Al_{13}Fe_4$ and $Al_{74}Co_{26}$ could be investigated at a few different temperatures in the undercooled regime and above the melting temperature. As an example, Fig 1a shows the structure factor, S(Q), determined for liquid $Al_{13}Fe_4$ at a temperatures of 1320K, which corresponds to an undercooling of 100 K. The pair correlation function g(r) corresponding to the S(Q) of Fig 1a is depicted in Fig 1b. The co-ordination number, Z, provides useful information on the SRO in liquids and it is usually estimated from the area under the first peak of $4\pi r^2 g(r)$. In the present case Z=11.7 was inferred. This coordination number is compatible with an icosahedral

SRO as well as with a SRO based on clusters with fcc or hcp structure, while a bcc-structure can be excluded. For a further analysis, S(Q) was simulated using a method described in [4] by assuming that tightly bound clusters with different structure exists in the melt. For $Al_{13}Fe_4$ liquids an excellent fit of the measured S(Q) at large wave vectors was obtained for an icosahedral SRO (see Fig. 1a), while the measured S(Q) cannot be described by a SRO with fcc, hcp or bcc structure. Therefore our experiments support the idea of an icosahedral SRO prevailing in metallic liquids.

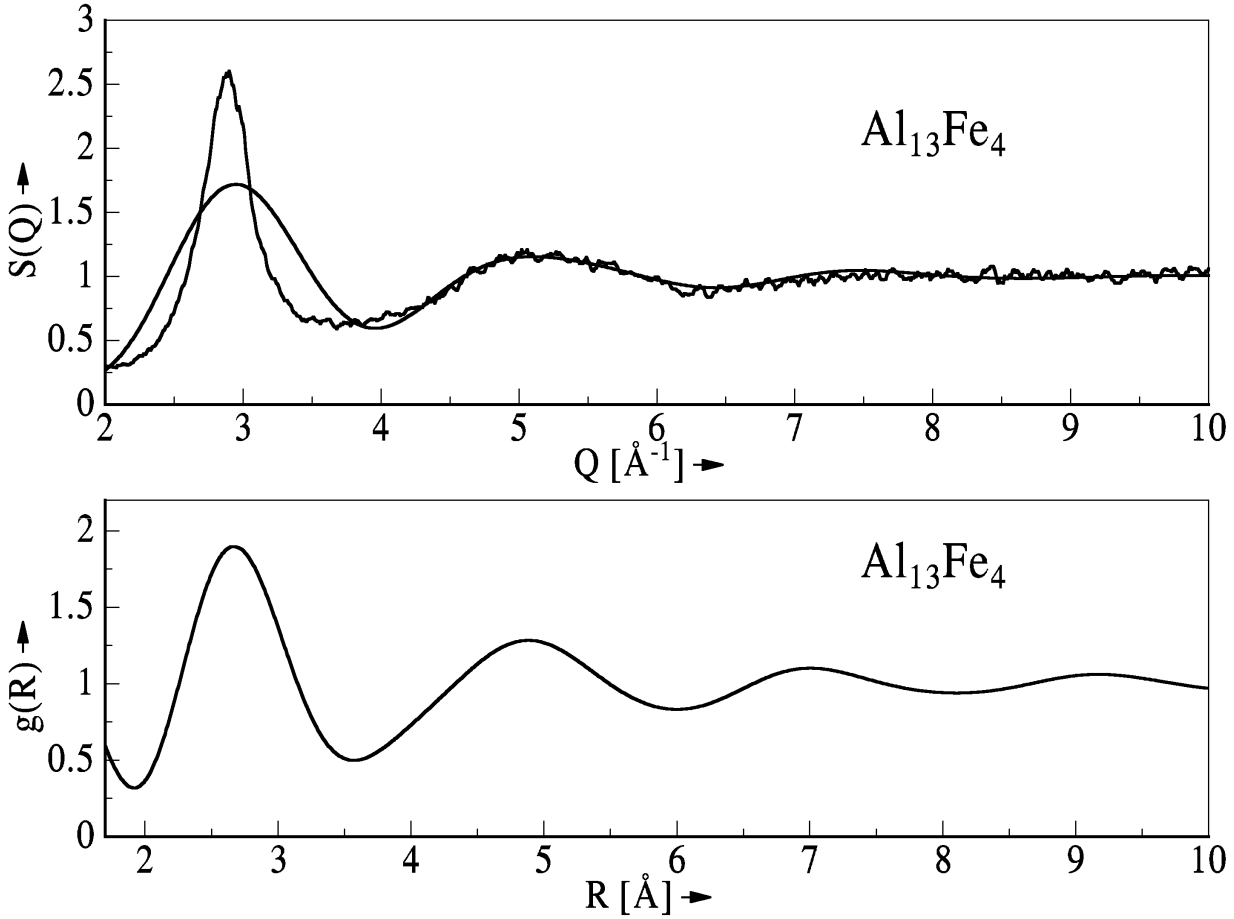

Fig. 1 Structure factor S(Q) for an Al13Fe4 melt undercooled by 100 K below its melting temperature and Simulation of S(Q) under the assumption of an icosahedral short-range order in the liquid (a) and corresponding pair correlation function g(R) (b).Fig1

References

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