ESRF	**Experiment title: Local order in AlMn and AlPdMn liquids forming quasicrystals**	**Experiment number:** HS-774
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Report:

Introduction : Stable quasicrystals exhibit both orientational order and long range quasiperiodic order. Their structure has been described as a packing of icosahedral units. For instance, in the case of the metastable icosahedral AlMn phase, the simplest icosahedral unit or cluster to be considered in a structural description is built from a transition metal atom surrounded by 12 atoms, mainly Al. Argument in favour of such a description is that the same cluster is also found in approximant periodic phases of the quasicrystal and that the cluster stability was proved by electronic density calculations (Gong X. et al., Phys. Rev. B **50**, 17701 (1994)). Besides, it has been proposed in different works that magnetic and electronic properties of solid phases would depend on this local icosahedral order (Simonet V. et al. Phys. Rev. B **58**, R8865 (1998) and Trambly de Laissardière et al., Phys. Rev. B **55**, 2890 (1997)).

Several neutron scattering experiments have already been performed in order to characterize the liquid structure in equilibrium with quasicrystalline or approximant phases (cf. Simonet V. et al., Phys. Rev. B **58**, 6273 (1998)). Indeed, liquids in equilibrium with these phases could also present an icosahedral local order at least just above the melting temperature and in the undercooled regime. The results obtained on AlPdMn and $Al_{88.5}(Mn_xCr_{1-x})_{11.5}$ liquid alloys revealed an overall similarity between the structure factor of both the solid and liquid states, thus suggesting the presence of a strong icosahedral local order above the melting point. Simulations of the large Q part of the structure factor from on a simple model of liquid containing a large proportion of icosahedral clusters show a very good agreement with the experimental results. Besides, such a local icosahedral order was also identified from the comparison between simulated and experimental partial pair distribution functions, obtained for the $Al_{88.5}(Mn_xCr_{1-x})_{11.5}$ ($0<x<1$) liquid alloys in which the isomorphic Mn/Cr substitution property was used. Moreover, the partial pair distribution functions in these liquids showed a strong chemical order with Mn atoms mainly surrounded by Al atoms. At last, icosahedral clusters seem to be still present at high temperatures in the liquid, though probably in weaker proportions. This yields the picture of a liquid containing rigidly bound atoms in icosahedral units.

Therefore, on the basis of such results, EXAFS experiments at the metal transition energy K edge were interesting to carry out, since the average local order around transition metal atoms might be identified by this technique and studied as a function of temperature.

Experimental section :

We performed last month an EXAFS experiment at the Mn K edge in transmission detection mode at the ID26 ESRF beam line on two AlMn liquids with Mn content of 11.5 and 3.5%. The signal has been obtained beyond the energy Mn K-edge (6.4 to 7.1 keV) in a quick EXAFS mode (regular displacement of the undulator gap). At each temperature (950 °C, 1100°C, 1300°C and 1500°C for $Al_{88.5}Mn_{11.5}$ and 1100 and 1300°C for $Al_{96.5}Mn_{3.5}$) around 100 EXAFS spectra have been recorded (10 h of counting) in order to get good statistics (1‰). The transmission factor of the whole set up with sample is less than 0.02%, but thanks to the high flux available on ID26, the data are of good quality.

Each sample was molten in a sapphire cell heated by a Mo furnace in a high temperature steel vessel. The choice of the sample holder has been motivated by the fact that AlMn liquids do not react with sapphire. The furnace and sapphire cell were built at the Laboratoire de Cristallographie (CNRS, Grenoble) where this sample conditioning is actually used to investigate fluids under high pressure and high temperature. The samples of about 50 µm thickness were inserted between two slices of sapphire. Note that upon melting, the samples kept their shape and did not flow down because of a thin natural oxide layer which remained unchanged during the experiment.

Results :

The EXAFS oscillations at the Mn K edge for the Al88Mn12 sample at 950 °C and 1500 °C are shown below. In addition to a decrease of the oscillations amplitude due to the increase of temperature, there may be an evolution of the phase of the oscillations (pointed out by the arrow). It could reveal the occurrence of Mn first neighbors at high temperature whereas just above the melting at 950 °C, Mn is only surrounded by Al atoms. This very preliminary result, that has to be checked by a thorough analysis of the oscillations, could give some insight in the magnetic properties of the AlMn liquids.