L-32 **Saturday, 18.06., 9^{00} - 9^{40}**

Investigating the structure of liquid metals at extreme conditions by X-ray absorption spectroscopy

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Keywords: liquid metals, x-ray absorption spectroscopy, high-temperature, high-pressure

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Investigating the structure of stable and undercooled liquids over a wide pressure range is an important issue in fundamental physics and represents an extraordinary experimental challenge with large implications in other fields, such as materials science and geophysics.

X-ray absorption spectroscopy (XAS) has the capability to provide atom specific information concerning interatomic distances and coordination numbers and, in favourable cases, beyond the pair correlations, on higher order distributions. For the analysis of liquids and disordered systems, a combination of molecular modelling methods and experimental data is essential to move beyond the traditional peak-fitting approach. For our studies, Reverse Monte Carlo (RMC) modelling has been implemented into XAS data analysis codes (RMC-GNXAS) [1] and provides realistic three dimensional models of the structure of disordered systems compatible with data sets from both XAS and diffraction experiments. Such models can then be analysed in terms of pair distribution functions, coordination numbers and bond angle distributions to obtain a complete insight into the atomic correlations at the microscopic level.

Within this contribution, some applications of XAS and Reverse Monte Carlo for the investigation of elemental liquid metals at ambient and high pressure conditions will be reviewed.

For liquid and undercooled Cu and Ni [2,3] at ambient pressure, signatures of short-range fivefold ordering have been investigated and estimates of the fraction of nearly-icosahedral configurations were obtained.

In the case of liquid Sn [4], the local coordination and geometry have been investigated up to moderate pressure (< 5 GPa) and related to the possible occurrence of pressure induced transitions between two different liquid phases (polyamorphism), largely debated for such metals involving directional and open coordination environments.

Recent experiments for the determination of the melting temperature of Fe at extreme pressure (up to the megabar) by XAS [5] will be also reported.

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