Probing Local Ordering in Liquid and Undercooled Metals by X-ray Absorption Spectroscopy

Trapananti A., Di Cicco A.[*] and Filipponi A.[1]

INFM, Dipartimento di Fisica, Università di Camerino, Via Madonna delle Carceri, I-62032 Camerino (MC), Italy (angela.trapananti@unicam.it)
[*]INFM and INFN-LNF, Dipartimento di Fisica, Università di Camerino, Via Madonna delle Carceri, I-62032 Camerino (MC), Italy
[1]INFM, Dipartimento di Fisica, Università dell'Aquila, Via Vetoio, I-67010 Coppito (AQ), Italy

A fundamental issue in the understanding of liquid matter regards its local structure. Local ordering in liquid condensed phases can be significantly different from that of corresponding crystalline systems. Signatures of five-fold local symmetries have been previously found in liquid metals but current knowledge is limited to the pair distribution, leaving considerable uncertainty in the determination of the geometrical structure.
The presence of specific local symmetries in liquid and deeply undercooled metal melts can be studied by taking advantage of an experimental technique such as x-ray absorption spectroscopy (XAS) which is sensitive to local higher-order correlations through multiple-scattering of the photo-excited electron from a core level.
Within this contribution, we will report about recent x-ray absorption experimental results on liquid and undercooled copper [1]. Experiments have been performed at the BM29 XAS beamline of the ESRF exploiting the opportunity to combine XAS, x-ray diffraction and single energy temperature scans [2]. Data have been interpreted using a novel Reverse Monte Carlo (RMC) method based on multiple-scattering simulations in order to provide a three-dimensional model of the disordered system compatible with the XAS data under consideration.
Results are shown to contain direct information on triplet correlations making feasible a reliable determination of the bond-angle distribution and fraction of icosahedral configurations in liquids.
Preliminary results for other liquid metals under extreme conditions will be also presented.

References

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