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Report:

Frank [1] predicted in 1952 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 short-range order (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 in this experiment the SRO of undercooled melts was investigated 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 and HS 800. Melts of Fe, Ni, Co-Pd and $Al_{13}Fe_4$ were studied by X-ray diffraction at different temperatures in the undercooled regime and above the melting temperature. Fig 1 shows the structure factor, S(Q), recorded for liquid Ni at temperatures of 1460K, 1530K, 1630K and at the melting point at 1726K. S(Q) measured for liquid Fe at temperatures of 1760K and at the melting point at 1809K is plotted in Fig 2. In the solid state iron shows a bcc structure at temperatures between 1667 K and the melting temperature of 1809 K while Ni has fcc structure. The pair correlation functions g(r) corresponding to the S(Q) of Fig 1 and Fig 2 are depicted in Fig 3. 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 $4\pi\rho r^2 g(r)$. In the present case $Z \approx 12$ was inferred for both elements at all temperatures. This 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] and assuming that one of these different SRO's exists in a melt in which tightly bound clusters are present (Fig 2). For both elements and all temperatures the best fit of the measured S(Q) was obtained for an icosahedral SRO.

References

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