# Structural Ordering in liquid AlMn and AlNi alloys

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The nature of the short-range structure is essential to understand the special properties of metallic liquids and glasses. With the discovery by Shechtman et al. [1] of quasiperiodic structures with icosahedral symmetry, many experimental attempts [2,3] have been made to study the local order in liquid alloys forming quasicrystalline phases such as based on Al-TM (TM= transition metal) alloys. For such alloys, the overall similarity observed between the structure factors of liquid phases and their parent icosahedrally coordinated quasicrystalline phases has been taken as the proof, albeit indirect, that the fivefold symmetry also exists over short range in the liquid phases.
Molecular dynamics simulations offer an alternate possibility to determine the short-range structure in liquids [4,5]. However, an accurate simulation of the properties of Al-TM alloys is still a challenging problem since bonding is not well described by currently available pair and embedded-atom potentials [6,7]. To further clarify the occurrence of the icosahedral short-range order (ISRO) in liquid Al-TM alloys, we have undertaken a study of structural properties of liquid $Al_{80}Mn_{20}$ and $Al_{80}Ni_{20}$ alloys based upon ab initio molecular-dynamics simulations.
The determination of the partial structure factors of both liquid alloys gives evidence of a pronounced chemical SRO, characterised by a strong Al-TM affinity. However, these results suggest also that the topological ordering extend over more interatomic distances in the liquid $Al_{80}Mn_{20}$ alloy. The fact that the topological short-range order is quite different in both alloys is also confirmed by bond angle distribution functions. A more refined structural analysis, using the common-neighbour analysis, giving a three-dimensional picture of the inherent structures from the simulations, allows us to emphasize the occurrence of a well pronounced ISRO in the liquid $Al_{80}Mn_{20}$ alloy.

**References**

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