NMR methods for investigation of complex metallic alloys

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Complex metallic alloys (CMA's) are intermetallic compounds characterized by (i) the large unit cells, comprising some tens up to thousands of atoms, (ii) the presence of well-defined atomic clusters, frequently of icosahedral point group symmetry and (iii) the occurrence of inherent disorder in an ideal structure [1]. In the last two decades there has been an increasing interest in CMA's due to the structural similarity of the atomic arrangement inside the unit cell with the short-range order structure of quasicrystals, which by definition have an infinite unit cell. This is why the CMA's are frequently referred to as approximants to the quasicrystals.

Because of the large size of the unit cell, the structural determination of CMA's is a complicated task. Diffraction methods are here an indispensable tool, whereas nuclear magnetic resonance (NMR) spectroscopy can offer complementary structural information on the local atomic scale [2-5]. The NMR spectra of quadrupolar nuclei such as ^{27}Al provide information on (i) the distribution of electric-field-gradient (EFG) tensors and the associated distribution of local atomic environments around the resonant nuclei, (ii) the number of crystallographically inequivalent lattice sites in the unit cell, and (iii) the local symmetry of the crystalline lattice. Various examples to demostrate the above aspects will be shown.

In addition, the ^{27}Al NMR experiments that prove a clathrate-like structure of Co_4Al_{13}, a traditional member of CMA's, will be presented. Recent X-ray investigation of high-quality single crystals in combination with theoretical calculations revealed a surprising analogy between Co_4Al_{13} [6] and

intermetallic clathrates. Co-Al-Co molecular groups play a role of the guest ions trapped in cages formed by other Al and Co atoms. Two ^{27}Al NMR lines were identified in Co_4Al_{13}. The first one originates from Al atoms forming cages. The second line corresponds to Al sites with exceptionally large, almost axially symmetric EFG tensor, in perfect agreement with the presence of isolated Co-Al-Co molecular groups [5].

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