Partial densities of electronic states in Al- or Mg-based complex intermetallics

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Soft X-ray emission spectroscopy (XES) is a unique technique that may be used to investigate separately Al s,d and Al p (Mg s,d and Mg p) states in solids of these elements with a very good energy resolution owing to the finite life time of the core hole created by electron excitation. It was extensively employed by Esther Belin-Ferré (EBF hereafter) with the aim to map both the valence and conduction sides of the electronic structure of selected complex compounds. The most salient results appeared out of a systematic study of quasicrystals (Al-Cu-Fe and Al-Pd-Mn) in comparison to crystals of related chemical composition, either binary compounds like θ-Al_2Cu or so-called approximants containing up to thousands atoms per unit cell.

In the interest of time, the talk will be restricted to a selection of the most important results of EBF, namely: i-evidence of the formation of a pseudo-gap at the Fermi energy in Al-based compounds and its correlation to the complexity of the atomic structure of the crystal (Fig. 1), ii-phase stability and transport properties of the same compounds in the light of the data gained about the Al-3p partial DOS, iii-formation and role on phase selection of d-states appearing close to, and below, the Fermi energy in Al- or Mg-containing compounds.

Accounting further for the lifetime achievements of EBF will not be possible in the context of this conference, but few key references[3,4] to her works will be provided.

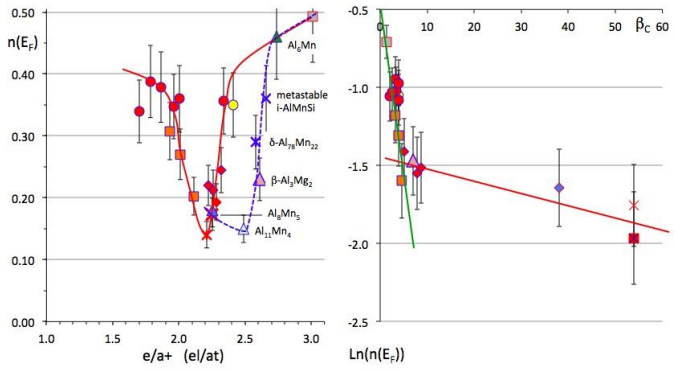

Fig. 1: Left: partial density of Al3p states measured by XES at the Fermi energy of a series of Al-Cu-Fe stable crystals and quasicrystals (data linked by a red line, to guide the eye) and binary Al-Mn and Al-Mg compounds (blue dashed line). The x-axis plots the e/a values corresponding to those compound compositions according to the e/a values for the individual constituents obtained by Mizutani and his co-workers[1]. Right: the same data in a log-log plot as a function of β_C=Ln(N_{UC}) where N_{UC} is the number of atoms per unit cell. The index β_C yields for a definition of the complexity of the lattice[2].

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3. Electronic structure in quasicrystalline compounds and related crystals
E. Belin-Ferré, J. of Phys. Condensed Matter **14** R789-R817 (2002).

2. Study of Al-Cu Hume-Rothery alloys and their relationship to the electronic properties of quasicrystals.
V. Fournée, E. Belin-Ferré, J. M. Dubois, J. Phys.: Cond. Matter **10** 4231-4244 (1998).

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