Oral Contributions

[MS19] Heavy crystals: structural crystallography of heavy-element compounds

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[MS19-01] Examples of Ordered or Disordered Ternary Intermetallics Containing Rare-earth Elements and Transition Metals

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In the first part of the presentation, the structural and magnetic properties of a new series of intermetallics with the general formula $RE_6M_{1.67}Si_3$ (RE = Ce-Tb, M = Co, Ni) [1-4] will be discussed. In these series $Gd_6Ni_{1.67}Si_3$ and $Gd_6Co_{1.67}Si_3$ exhibit very interesting magnetocaloric effect with the existence of an important magnetic entropy variation ΔS_m around room temperature [3]. All these compounds crystallize with the $Ce_6Ni_{1.67}Si_3$ structure type [2]. This structure type is closely related to the $Ho_4Co_{3.07}$ (or $Ho_6Co_{4.61}$) structure type [5] with a perfect ordering between silicon and cobalt/nickel atoms. This hexagonal structure (S.G. $P6_3/m$) is characterized by infinite chains of face-shared trigonal prisms [RE_6] filled by Si or M atoms. Theses chains are running along the c-axis and extend as triangular columns by sharing rectangular faces in the (a, b)-plane. Between these columns infinite chains of face-shared [RE_6] octahedra are partially filled by M-atoms (Fig. 1). The strong delocalization of the electron density of M-atoms observed in these latter chains has been attributed to strong steric strains (Fig 1). This behavior was also observed in the homologous binary compound $Gd_6Co_{4.85}$ [6].
In the second part, the discovery of two new Mg-rich phases in ternary systems RE-M-Mg (RE = La, Gd, and M = Ni, Cu) will be presented. $LaCuMg_8$ [7] crystallizes in the La_2Mg_{17} structure type (S.G. P63/mmc) with the lattice parameters a = 10.1254(2) and c = 10.0751(2) Å. A disordered structure is observed with a random distribution of Cu atoms on some La and Mg positions. The structure of the second phase, $Gd_{13}Ni_9Mg_{78}$ [8], was not fully determined because of a medium crystallinity. The structure was partially deduced using TEM and an average cubic structure with lattice parameter a = 4.55 Å could be assumed. A modulation along both **a*** and **b*** axis with vectors of modulation q1 = 0.42**a*** and q2 = 0.42**b*** was observed. Because of the high amount of magnesium, the hydrogen absorption properties of these new phases were studied.

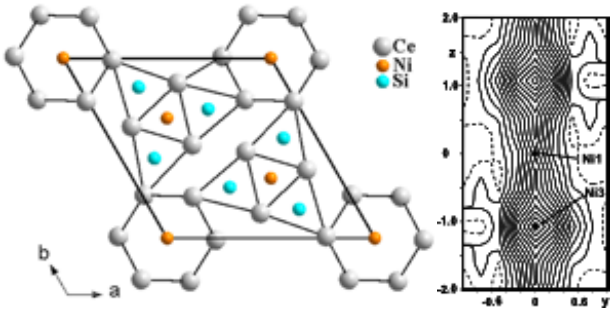

Figure 1: Structure of $Ce_6Ni_{1.67}Si_3$. Left: Projection along the c-axis. Right: Fourier-map showing the strong delocalization of the electron density within the chains of face-shared octahedra

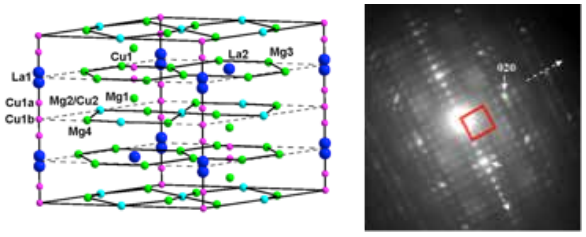

Figure 2: Left: Structure of $LaCuMg_8$. Right: Electron diffraction pattern of $Gd_{13}Ni_9Mg_{78}$

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