Magnetic short range order in $Fe_{1-x}Cr_x$ alloys

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FeCr alloys now encounter high interest due to their ability to eliminate irradiation damages spontaneously at high temperature. This property makes them crucial ingredients in future fusion and fission reactors, where materials suffer extensive damage from high energy neutrons irradiation. The unique stability of FeCr is likely related to an inversion of atomic short range order (SRO) at x_c=0.11 [1,2], and to a sign inversion of the heat of formation [3]. Below x_c, the Cr atoms repel each other, leading to ordering, whereas above x_c they tend to cluster. Such inversion is theoretically explained by the influence of band ferromagnetism on the atomic interactions, leading to a change of sign of the atomic pair potential with Cr content [4].

In FeCr alloys, chemical and magnetic local orders are strongly coupled. To investigate this coupling, we studied $Fe_{1-x}Cr_x$ bcc solid solutions (for 0.03<x<0.15) by neutron diffuse scattering, using both polarized and unpolarized neutrons. Polycrystalline alloys were annealed to ensure equilibrium SRO states [2]. At low Cr content, the Cr moment orients anti-parallel to the Fe moment, with a value of -1.14(1) μ_B. The Cr moment perturbs the neighboring Fe moments, decreasing their magnitude for the near Fe neighbors and increasing it for farther Fe neighbors. At high Cr content, the Cr moment decreases, being strongly sensitive to the number of Cr neighbors.

These results extrapolate well with *ab initio* predictions performed in the dilute limit [5], for the amplitude and sign of the local moments and perturbations (Figure). At high Cr content, the decrease of the Cr moment is qualitatively explained by magnetic frustration effects [6]. New DFT calculations coupled with MC simulations are now in progress to evaluate the moments and perturbations for the actual SRO states. The whole study brings out the pivotal role of magnetism in iron defects, a key feature to control the design of steel materials for fusion energy [7].

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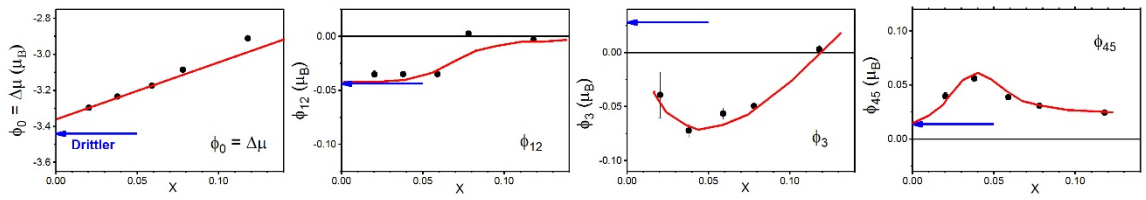

Figure 1: Moment difference (μ_{Cr}-μ_{Fe}) and magnetic perturbations of Fe moment due to the presence of a Cr atom in the nearest neighbor shells. Experimental results are compared to the predictions of [5] using LDA-DFT *ab initio* calculations in the single-impurity limit (blue arrow).