Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Local hyperfine field systematic of sp impurities on (001) and (111) Ni Surfaces MARCUS TOVAR COSTA, Universidade do Estado do Rio de Janeiro, Instituto de Aplicacao, Brazil, ALEXANDRE DE OLIVEIRA, Centro Federal de Educacao de Quimica de Nilopolis, Brazil — A self-consistent calculation of the local magnetic moments and the hyperfine fields is performed, considering a systematic of n-*sp*, (n=4,5) impurities on (001)Ni and (111)Ni surfaces and sublayers. A simple model is adopted which is, in principle, an extension on that of Daniel and Friedel. The behavior obtained for the hyperfine fields for each one of the series namely above is drastically different from that obtained for the bulk. The calculations of the electronic structure of the systems are based on a full multi-orbital tight-binding model and using the Green function formalism. The effect of next-neighbor perturbation on the magnetic properties, due to the lost of translational invariance introduced by the impurity, is taken into account in the present picture. The theoretical results are in agreement with known experimental data.

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Date submitted: 25 Nov 2008 Electronic form version 1.4