EXCHANGE STIFFNESS PARAMETER AND MAGNETIZATION IN PSEUDOPOTENTIAL CALCULATIONS

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9.7 cm

A spin dependent pseudopotential is determined by the Hohenberg-Kohn formalism and the local spin density approximation. The spontaneous magnetizations are calculated for uniform spin densities of valence electrons and in the Lindhard approximation. The stiffness parameter of the Landau-Kittel Hamiltonian (Bloch wall parameter) is obtained in the Bragg-Williams approximation. *Ab initio* numerical results of the magnetization and the exchange stiffness parameter are shown in Table, for *bcc* Fe, *fcc* Co and Ni. The intention of this article is to show what can be found concerning magnetic properties, by means of a simple approach.

Table: Magnetic moments per Wigner-Seitz cell in Bohr magneton. The calculated moments: S_{uni} and S_{Lin} are for uniform valence spin gas and in the Lindhar approximation, respectively. The experimental literature moments are denoted by S_{expt} . The calculated and experimental exchange stiffness parameters, A_{cal} and A_{expt}, are multiplied by the volume, V_{ws}, of the Wigner-Seitz cell (in the atomic units [a.u.]).

$3d$ metal	S_{uni}	S_{Lin}	S_{expt}	$A_{cal}V_{ws}[a.u.]$	$A_{expt}V_{ws}[a.u.]$
Fe [*bcc*]	2.0	2.5	2.22	0.073	0.041
Co [*fcc*]	1.8	1.6	1.68	0.031	0.034
Ni [*fcc*]	0.97	0.9	0.60	0.020	0.014

13.4 cm

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