Hyperfine fields of S-rare earth impurities in noble hosts

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Hyperfine fields of S-rare earth impurities in noble hosts

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Résumé. — Le champ hyperfin d'auto-polarisation d'impuretés de Gd^{3+} et Eu^{2+} dans les matrices nobles est calculé à partir du modèle simple développé pour les impuretés de terre rare dans les matrices s-p [1]. Les résultats numériques sont obtenus en fonction du paramètre d'hybridization d'Anderson-Moriya (AM). Les résultats expérimentaux peuvent être décrits par notre modèle. Les impuretés divalentes de Eu^{2+} dans les métaux nobles sont décrites par une bande perturbée à la Slater-Koster (SK) et la résonance d'un état d presque vide.

Abstract. — The self-polarization hyperfine field of Gd^{3+} and Eu^{2+} impurities in noble hosts is calculated using an extension of a simple model previously developed for rare earth impurities diluted in s-p hosts [1]. Numerical results for the hyperfine field for increasing bandwidths (from Cu to Au) and several strengths of the phenomenological Anderson-Moriya (AM) hybridization parameter are presented. Experimental results can be understood within our picture. Eu^{2+} impurities in noble metals could be described by a Slater-Koster (SK) perturbed conduction band and an almost empty d-resonance hump.

Theoretical studies of the self-polarization hyperfine field of rare earth impurities in s-p and transition hosts have been made in previous works [1, 2]. Concerning transition hosts [2] the main effects are the strong one-electron perturbation associated to the charge difference between host and impurity and the local change of the Coulomb interaction at the impurity site [2]. These effects are at the origin of the almost equal values for the hyperfine constants of these impurities placed in 4d or 5d hosts [3].

In the case of s-p hosts, it is suggested that the trivalent rare earth impurities acts in two ways. (i) They introduce a strong repulsive potential which locally deforms the s-p conduction band; (ii) The d-state associated to the rare earth resonates over this deformed s-p conduction band thus producing a virtual bound state [1]. Contrary to the transition host case, there is a possibility of a change in sign of the hyperfine field along the s-p series.

Concerning noble metals, the virtual bound state picture has been invoked previously in the literature to explain anomalous Hall effect [4]. It is known experimentally that Er diluted in Ag and Au hosts exhibit almost the same positive value for the hyperfine constant.

We have applied the model developed in [1] to the noble host case. An essential difference concerning the SK perturbation occurs in this case as compared to s-p metals. In fact, assuming that the trivalent rare earth (e.g. Gd^{3+}) contributes two s-p electrons, for monovalent hosts like noble metals, the Slater-Koster (SK) potential is an attractive one.

Concerning the host, available band calculations [5] suggest that the unfilled (s-p) part of the conduction states may be approximately represented by a Moriya-like parabolic density of states. We adopt Campbell's picture [6] of eight identical subbands; the half-widths Δ_c of these are 2, 3 and 4 eV for Cu, Ag and Au respectively (period effect). From the band calculations it is expected that host s-d hybridization increases in going from Cu to Ag and one expects it still increases for Au [5]. The main lines of the model go as follows cf. [1]. The SK attractive potential (V_{cc}), which perturbes the density of states is determined via Friedel's sum rule. Concerning the d-resonance, the position of the *atomic level* (ε_d) relative to the Fermi energy (ε_f) is calculated self-consistently using the extended Friedel sum rule [1].

The local exchange interaction with the 4f-level, is treated in the Born approximation and one obtains the self-polarization hyperfine field in terms of the local magnetic responses [1].

The total hyperfine field for each host, as a function of the strengh of the hybridization $| V_{cd} |^2$ (the only free parameter of the model) is shown in figure 1. The ratio $J^{(d)} A_{cp}^{(d)}/J^{(c)} A(Z)$ is taken fixed and equal to 0.5 as discussed in [1] and [2]. $J^{(c)}$ and $J^{(d)}$ are the exchange couplings between the localized 4f spins and the s-p conduction states and d-resonance states respectively. $A_{cp}^{(d)}$ and $A(Z)$ are the induced d-core hyperfine constant and the contact hyperfine constant respectively.

We note that the d-f exchange coupling $J^{(d)}$ is taken to be positive, in contrast to the case of hosts exhibiting strong d-character [2]. We have changed the $J^{(d)}/J^{(c)}$ ratio from 2 to 1 and the effect on the total hyperfine field is only about 15 %. From the results ploted in figure 1, one sees that the region of positive

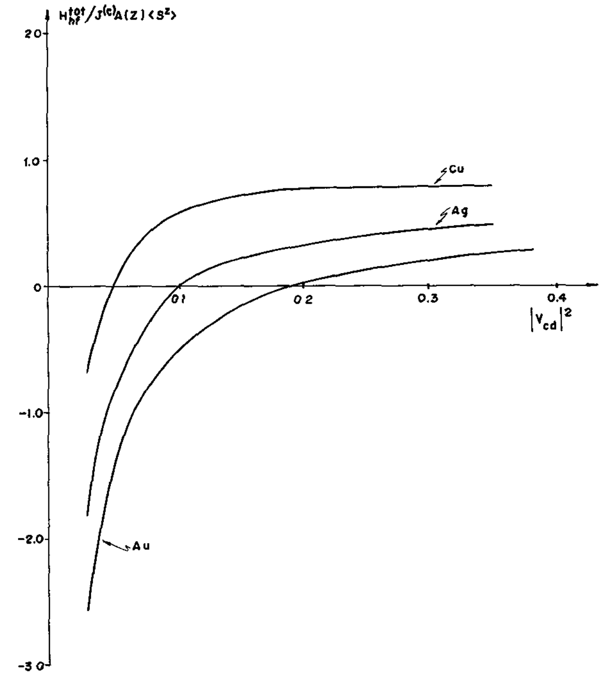

Fig. 1. — Self-polarization field of Gd^{3+} (in units of $J^{(c)}A(Z)\langle S^z\rangle$) as a function of $|V_{cd}|^2$ for Cu, Ag and Au hosts (see text).

self-polarization fields corresponds to increasingly higher $|V_{cd}|^2$ matrix elements when one goes from Cu to Au. This is in agreement with the increasing host value of the s-d hybridization if $|V_{cd}|^2$ is interpreted as in [7], i.e., the Anderson-Moriya (AM) resonance being associated to host hybridization. From experiments performed in Er$\underset{\sim}{\text{Ag}}$ and Er$\underset{\sim}{\text{Au}}$ systems one may estimate from figure 1 that the appropriated values of $|V_{cd}|^2$ for Ag and Au are roughly 0.12 eV and 0.21 eV respectively.

Now concerning divalent rare earth impurities, such as Eu^{2+}, one would expect for the total self-polarization hyperfine field the behavior depicted in figure 2. In fact, for divalent Eu in the absence of occupied d-states, only the SK perturbation remains and the field is always positive. We have plotted the total hyperfine field as a function of the half band-width, since $|V_{cd}|^2$ plays no relevant role in this case. The trend showed in figure 2 is understandable since for larger bandwidths the local magnetic responses should decrease. One predicts

$$H_{hf}(\text{Au})/H_{hf}(\text{Ag}) \cong 0.5 ,$$

i.e., an appreciable period effect occurs, contrary to the case of trivalent impurities. So, experimental results could be very interesting to check this model.

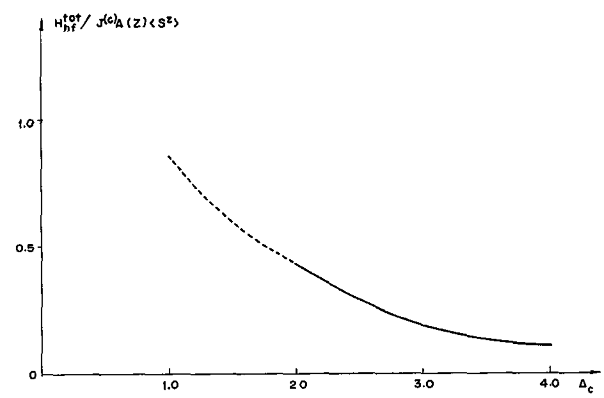

Fig. 2. — Self-polarization field of Eu^{2+} (in units of $J^{(c)}A(Z)\langle S^z\rangle$) as a function of the band width of the host (see text).

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