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Comments and Addenda

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ESR linewidth of rare-earth ions in dilute rare-earth alloys

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The exchange coupling between the $4f$ magnetic electrons and the $5d$-like screening electrons is calculated for Er and Dy dilute magnetic alloys, in the limit that the strength of the spin-orbit coupling of the $5d$ virtual bound state is much greater than its half-width. Significant cancellation between the spin and orbital components of the exchange is found. This leads to a drastic reduction in the calculated linewidth from the value calculated in the absence of spin-orbit coupling.

In a recent paper we have calculated the exchange coupling between the $4f$ electrons and the $5d$-like screening electrons in dilute rare-earth alloys.[1] This coupling was shown to be anisotropic with significant orbital contributions. We have derived the g shift and thermal linewidth of the rare-earth ion for the case that the strength λ of the spin-orbit interaction of the $5d$ virtual bound state (VBS) is much less than its half-width Δ. Hence we could ignore the splitting of the $5d$ VBS by the spin-orbit interaction. Our calculated value for Δg and $\Delta H/\Delta T$ are in good agreement with experiments for the Γ_7 doublet of Er and Dy in Al host, where Δ is known to be large (~2 eV). It was pointed out to us by Fert[2] that if our expression for the linewidth[3] is applied to rare-earth ions in noble metals, where Δ is known to be much less (~0.5 eV),[4] one would get an unreasonably large linewidth (~140 G/K for Γ_7 doublet of Er). In this paper we wish to show that if λ is greater than or comparable to Δ (the latter is the case in noble metals), the splitting of the $5d$ VBS by the spin-orbit coupling leads to a partial cancellation between the spin component and the orbital component of the exchange. Consequently, the calculated linewidth is reduced, bringing the theory back into rough agreement with the experiment.

In dilute rare-earth alloys, λ is known to be positive (~0.1 eV),[5] so that the lowest-lying $5d$ states can be represented by $j=\frac{3}{2}$ with an excited $j=\frac{5}{2}$ manifold roughly 0.3 eV above. For simplicity, we consider the extreme case $\lambda \gg \Delta$ so that one can neglect the density of states at the Fermi level from the $j=\frac{5}{2}$ states. Further, we consider only the spin and orbital components of the exchange interaction of the form

$$\mathcal{H}_{ex} = -a_0 \vec{S}\cdot\vec{s} - a_1 \vec{L}\cdot\vec{l} \,. \tag{1}$$

Projecting $\vec{S}$ and $\vec{L}$ onto the effective spin $\vec{\tilde{S}}$ appropriate to the rare-earth multiplet, and replacing $\vec{s}$ by $(g_j-1)\vec{j}$ and $\vec{l}$ by $(2-g_j)\vec{j}$ for the $5d$ VBS, we can rewrite the exchange coupling as

$$\mathcal{H}_{ex} = -J_{eff}\, \vec{\tilde{S}}\cdot\vec{j} \,. \tag{2}$$

For $j=\frac{3}{2}$ $(=l-s)$, we find a significant cancellation between the spin and orbital components. Using

TABLE I. Exchange interaction appropriate to a Γ_7 doublet.

	Spin component	Orbital component	J_{eff}
Er	720	−679	41
Dy	591	−1118	−527

our estimates for the exchange integrals,[1] we list the exchange interaction appropriate to a Γ_7 doublet in Table I (in units of cm^{-1}). The contribution of the exchange coupling (2) to the thermal linewidth can be calculated in a straightforward way. We find

$$\Delta H/\Delta T = 10\pi k N_{3/2}^2 J_{\text{eff}}^2 / g\mu_B , \qquad (3)$$

where $N_{3/2}$ is the conduction electron density of states (per each m_j state) at the Fermi level with $j=\frac{3}{2}$. For the case that only $j=\frac{3}{2}$ states are appreciably occupied, $N_{3/2}$ is simply given by $1/2\pi\Delta$. Using $\Delta \simeq 0.5$ eV, we find $\Delta H/\Delta T$ equal to 0.2 G/K for Er and 26.7 G/K for Dy. When compared to our previous results, these values for $\Delta H/\Delta T$ exhibit a drastic reduction. The experimental linewidths are found to be 10.5 G/K for Ag:Er,[6] 2.7 G/K for Au:Er,[7] and 18.5 G/K for Ag:Dy.[8] A realistic calculation for these systems must take into account $j=\frac{5}{2}$ states and the crystal-field splitting. Obviously, such calculations will be quite involved.

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[1]N. L. Huang Liu, K. J. Ling, and R. Orbach, Phys. Rev. B 14, 4807 (1976).

[2]A. Fert (private communication); also, A. Fert and P. M. Levy, Phys. Rev. B (to be published).

[3]Reference 1, Eq. (18).

[4]S. Hufner, G. K. Wertheim, and J. H. Wernick, Sol. State Commun. 17, 1585 (1975).

[5]A. B.Callender and S. E. Schnatterly, Phys. Rev. B 7, 4385 (1973).

[6]R. Chui, R. Orbach, and B. L. Gehmann, Phys. Rev. B 2 2, 2298 (1970).

[7]E. P. Chock, D. Davidov, R. Orbach, C. Rettori, and R. J. Tao, Phys. Rev. B 5, 2735 (1972).

[8]S. Oseroff, M. Passeggi, D. Wohlleben, and S. Schultz (unpublished).