CRYSTAL FIELD EFFECTS IN THE ESR SPECTRA OF RARE-EARTHS IN THE INTERMEDIATE VALENCE COMPOUND $CePd_3$

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ESR experiments reported on $CePd_3$ doped with magnetic rare-earths (Gd, Dy) (1,2) were published together with qualitative interpretations by their authors. Quantitative understanding of the data requires theoretical calculation, which is different for S (Gd^{3+}) and non-S (Dy) ground state ions. We were able, and report here, to get a complete fitting of those published spectra, which allows us to obtain quantitatively the relevant parameters in both cases.

First, we shall discuss the $CePd_3$ Gd system. Experiments made on single crystals (1) allow one to observe an almost resolved fine structure of Gd^{3+} at 1.6 K. This structure narrows at higher temperatures. Following Plefka (3) we used the projector's formalism in order to calculate the transverse susceptibility of the system, which is obtained through perturbation theory applied to the transition matrix. Spin-spin interaction was included phenomenologically. Details of the calculation will be published elsewhere. After fitting the low temperature spectra, we found necessary to include the IV effect in order to explain the non-linear behavior of the Gd^{3+} spectra at high temperatures ($T > 70$ K). The collapsed line broadens exponentially, which could be explained considering an excitation energy between Ce configurations. This phenomenological parameter, E_{ex}, could be fitted to be 400 K, in good agreement with other experiments in $CePd_3$. Other relevant parameters obtained were the fourth order crystal field, $b_4 = 23$G the Korringa thermal broadening $b = 0.45$ G/K.

Let us secondly analise the $CePd_3$:Dy system. This system shows and excited Γ_7 a few degrees above an anisotropic ground state. We included in our Hamiltonian the Zeeman effect, cubic crystal field, exchange interaction of the localized momenta with the conduction electrons, and a random distribution of strains in the sample. We diagonalized the Hamiltonian altogether, and calculated the spectra as a function of the temperature. The anisotropy of the Γ_8 lines was introduced in the same way as reported by Barberis (4). We obtained two crystal field parameters $W = .25$ and $x = 0.62$. Also relevant parameter is the Korringa thermal broadening of the Γ_7 and Γ_8 levels, $b = 1.5$ G/K. The simulated spectra and details of the calculation will be reported elsewhere, because of lack of space. The same is for $CePd_3$:Er. Summarizing, we could reproduce completely the ESR spectra of rare-earths in $CePd_3$. Crystal field parameters, and the excitation energy for the $4f^0 \leftrightarrow 4f^1$ configurations of Ce could be obtained with very good precision. This technique can be applied to other systems.

REFERENCES

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