acta phys. slov. 31. (1981), No. 2—3

THE INFLUENCE OF THE CRYSTAL FIELD ON THE PARAMAGNETIC SUSCEPTIBILITY OF $PrCu_2$ [1]

ВЛИЯНИЕ ВНУТРИКРИСТАЛЛИЧЕСКОГО ПОЛЯ НА ПАРАМАГНИТНУЮ ВОСПРИИМИЧНОСТЬ $PrCu_2$

Š. ZAJAC*, Prague

The energy levels and the eigenfunctions resulting from the splitting of the $^3H_4$ ground term of Pr^{3+} ions in the orthorhombic crystal field of $PrCu_2$ have been determined. Using these quantities the paramagnetic susceptibility of $PrCu_2$ has been calculated. A significant deviation from the Curie–Weiss law in the temperature dependence of paramagnetic susceptibility below 200 K has been found.

Previous investigations on the series of the rare-earth copper compounds with the orthorhombic $PrCu_2$ structure [1—3] have shown large magnetic anisotropy of these materials which is still present in the paramagnetic temperature range. Hashimoto et al. [3] have introduced a description of the crystal field in these compounds as the basis for the explanation of the observed anisotropy of their paramagnetic Curie temperatures. The aim of our work has been to calculate the influence of the crystal field in these compounds on their paramagnetic susceptibility for which the deviations from the Curie–Weiss law have been found experimentally.

We have approximated the crystal field Hamiltonian by two main terms

$$H_c = V_2^0(3J_z^2 - J(J+1)) + V_2^2\frac{1}{2}(J_+^2 + J_-^2), \qquad (1)$$

where V_2^0 and V_2^2 are the crystal field parameters and J is the total angular momentum of the rare earth ion in the RCu_2 compound. We have performed calculations for the compound $PrCu_2$ for which the paramagnetic phase is observed only and its crystal field parameters were determined by the following values [3]: $V_2^0 = 5.9\times10^{-10}$ J/ion, $V_2^2 = 4.1\times10^{-21}$ J/ion. Choosing the matrix elements of the considered crystal field Hamiltonian according to [4] we have made numerical diagonalization of the crystal field matrix. The ground term of the Pr^{3+} ion is $^3H_4$. In the given crystal field the ninefold degenerated $^3H_4$ term splits into nine singlets. The computed energy levels and the corresponding eigenvectors of the crystal field states are given in Table 1.

The paramagnetic susceptibility per ion has been calculated from the Van Vleck formula

$$\chi_i(T) = g^2\mu_B^2\left(\sum_n e^{-E_n/kT}\right)^{-1}\left(\sum_n \frac{|M_{nn}|^2}{T} e^{-E_n/kT} + 2\sum_{n\neq n'} \frac{|M_{nn'}|^2}{E'_n - E_n} e^{-E_n/kT}\right). \qquad (2)$$

---

[1] Contribution presented at the 6th Conference on Magnetism in Košice, September 2—5, 1980.

* Faculty of Mathematics and Physics of the Charles University, Ke Karlovu 3, CS-121 16 PRAGUE 2.

Table 1

Energy levels and eigenvectors of the $^3H_4$ ground term in the orthorhombic crystal field of $PrCu_2$

energy ($\times 10^{-21}$ J/ion)	eigenvectors
167.51	$0.703\|4\rangle + 0.075\|2\rangle + 0.020\|0\rangle + 0.075\|-2\rangle + 0.703\|-4\rangle$
167.39	$-703\|4\rangle - 0.071\|2\rangle + 0.071\|-2\rangle + 0.703\|-4$
50.91	$-0.678\|3 \ -0.200\|1\rangle - 0.200\|-1\rangle - 0.678\|-3\rangle$
46.93	$-0.697\|3\rangle - 0.120\|1\rangle + 0.120\|-1\rangle + 0.697\|-3\rangle$
−19.14	$-0.072\|4\| + 0.615\|2\rangle + 0.484\|0\rangle + 0.615\|-2\rangle - 0.072\|-4$
−49.39	$0.071\|4\rangle - 0.703\|-2\rangle + 0.703\|-2\rangle - 0.071\|-4$
−68.91	$-0.200\|3 \ +0.678\|1\rangle + 0.678\|-1\rangle - 0.200\|-3\rangle$
−146.93	$-0.120\|3\rangle + 0.697\|1\rangle - 0.697\|-1\rangle + 0.120\|-3\rangle$
−148.36	$0.024\|4\rangle - 0.341\|2\rangle + 0.875\|\| - 0.341\|-2\rangle + 0.024\|-4$

Here g is the Landé factor, μ_B is the Bohr magneton and k and T denote the Boltzmann constant and temperature, respectively. The matrix elements $M_{nn'}$ are defined as $M_{nn'} = \langle n/J_i/n' \rangle$, where J_i is the component of the total angular momentum in the i-direction of the applied magnetic field and $|n\rangle$ denote the different crystal field eigenstates with energies E_n.

The calculated temperature dependence of the inverse susceptibility along the principal crystalline b — axis $\chi_b^{-1}(T)$ for $PrCu_2$ is given in Fig. 1. It has been found that the deviation from the linear behaviour of $\chi_b^{-1}(T)$ for $PrCu_2$ begins below 200 K and is most remarkable below 100 K. For quantitative comparison it would be necessary to measure the paramagnetic susceptibility of $PrCu_2$ in the full temperature range mentioned above.

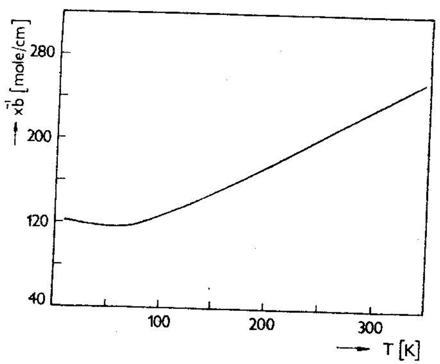

Fig. 1. Temperature dependence of the inverse susceptibility along the crystalline b-axis of the $PrCu_2$ compound.

REFERENCES

[1] Sherwood, R. C., Williams, H. J., Wernick, H. J.: J. Appl. Phys. *35* (1964), 1049.

[2] Ott, H. R., Andres, K., Wang, P. S., Wong, Y. H., Lüthi, B.: *in Crystal Field Effects in Metals and Alloys* (Ed. A. Furrer) Plenum Press, New York, London 1977.

[3] Hashimoto, Y., Fujii, H., Fujiwara, H., Okamoto, T.: J. Phys. Soc. Jap. *47* (1979), 67.

[4] Hutchings, M. T.: Solid State Physics *16* (1964), 227.

Received October 13th, 1980