The influence of the crystal field on the anisotropic thermal expansion in $TmCu_2$

1993 J. Phys.: Condens. Matter 5 7955

(http://iopscience.iop.org/0953-8984/5/43/009)

J. Phys.: Condens. Matter 5 (1993) 7955–7958. Printed in the UK

The influence of the crystal field on the anisotropic thermal expansion in $TmCu_2$

E Gratz, A Lindbaum and M Rotter

Institute for Experimental Physics, TU Vienna, Wiedner Hauptstrasse 8–10, A-1040 Vienna, Austria

Received 21 May 1993, in final form 24 August 1993

Abstract. The lattice parameters a, b and c of $TmCu_2$ have been measured in the temperature range from 4.2 K up to 300 K using x-ray powder diffraction. The influence of the crystal field on the thermal expansion in $TmCu_2$ in the paramagnetic region has been determined by comparing the thermal expansion of the non-magnetic YCu_2 with that of $TmCu_2$ ($TmCu_2$ orders magnetically at $T_N = 6.3$ K). The data thus obtained are compared with a theoretical model given by Gratz *et al* in 1993 using a set of crystal field parameters published by Gubbens *et al* in 1992. From this analysis we get information about the unknown elastic and magnetoelastic properties of $TmCu_2$.

1. Introduction

The aim of this paper is to show the crystal-field (CF) influence on the temperature variation of the lattice parameters a, b and c of $TmCu_2$ (orthorhombic $CeCu_2$ structure) in the temperature range from 4.2 K to 300 K by comparison with the isostructural YCu_2. Recently Gubbens *et al* [2] published a set of CF parameters for this compound determined from neutron scattering data, measurements of the magnetization, specific heat and thermal expansion. The aim of this paper is to apply this set of parameters to analyse the anisotropic thermal expansion for $TmCu_2$ (Tm^{3+} : $J = 6$) as it has been done in our recent publication for $ErCu_2$ and $NdCu_2$ (see Gratz *et al* [1]).

2. Experimental details

Polycrystalline samples of $TmCu_2$ and YCu_2 have been prepared by induction melting under a protective argon atmosphere. After annealing at 700 °C for one week no trace of foreign phases could be observed by the x-ray analysis.

A conventional Siemens D-500 x-ray powder diffractometer with an Oxford helium-flow cryostat and Co Kα radiation has been used for the measurements of the lattice parameters a, b and c as a function of temperature. Germanium was used as an internal standard for calibration at each temperature.

3. Results and discussion

The temperature variation of the lattice parameters a, b and c of $TmCu_2$ and YCu_2 is shown in figure 1. In order to make the comparison easier we normalized the lattice

0953-8984/93/437955+04$07.50

parameters to 300 K, that is, we divided them by the values at 300 K. The values of YCu_2 are given by the different broken lines in this figure. The lattice parameters at 300 K for $TmCu_2$ are $a = 4.267 \pm 0.001$ Å, $b = 6.713 \pm 0.003$ Å, $c = 7.248 \pm 0.001$ Å and for YCu_2 $a = 4.301 \pm 0.001$ Å, $b = 6.874 \pm 0.003$ Å, $c = 7.297 \pm 0.001$ Å.

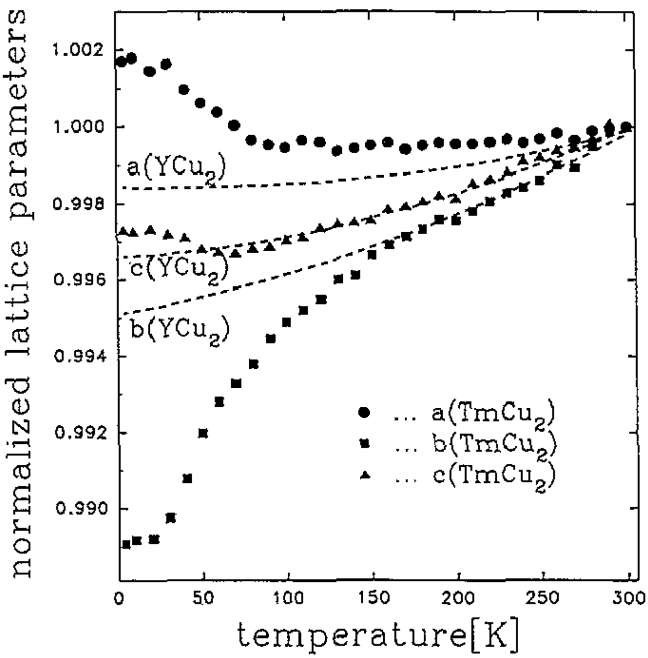

Figure 1. Temperature dependence of the normalized lattice parameters of $TmCu_2$ (symbols) and YCu_2 (broken lines).

The measured variations of $a(T)$, $b(T)$ and $c(T)$ for $TmCu_2$ deviate remarkably from those of the isostructural YCu_2 compound. The experimentally determined differences of the normalized lattice parameters of $TmCu_2$ and YCu_2 in the temperature range from 4.2 K to 300 K are shown in figure 2. As in our previous paper [1] we attribute the anomalous behaviour in the anisotropic thermal expansion of $TmCu_2$ to the CF influence.

If $a_i(T)$ $(i = 1, 2, 3)$ denotes the lattice parameters a, b and c of the magnetic compound $TmCu_2$ and $r_i(T)$ the lattice parameters of the non-magnetic isostructural compound YCu_2, the difference of the lattice parameters (normalized to $T_n = 300$ K) is given by (10) in [1]:

$$\frac{a_i(T)}{a_i(T_n)} - \frac{r_i(T)}{r_i(T_n)} = A_i(\langle O_2^0\rangle_T - \langle O_2^0\rangle_{T_n}) + B_i(\langle O_2^2\rangle_T - \langle O_2^2\rangle_{T_n}). \qquad (1)$$

Here the $\langle O_l^m\rangle_T$ and $\langle O_l^m\rangle_{T_n}$ denote the expectation values of the Stevens operators with $l = 2$ an $m = 0, 2$ at the variable temperature T and at the normalization temperature T_n (= 300 K), respectively. The CF parameters recently determined by Gubbens *et al* [2] (see also table 1) have been used for the calculation of the thermal expectation values of the Stevens operators. The coefficients A_i and B_i, which include elastic and magnetoelastic properties of the compounds are fitted to the experiment (for more details see our recent paper [1]). The obtained values for the six unknown coefficients are: $A_1 = 5.9\times10^{-5}$, $A_2 = -1.1\times10^{-4}$, $A_3 = 1.1\times10^{-5}$, $B_1 = 2.1\times10^{-4}$, $B_2 = -3.9\times10^{-5}$ and $B_3 = -6.6\times10^{-5}$.

The curves in figure 2 show the results of the calculation.

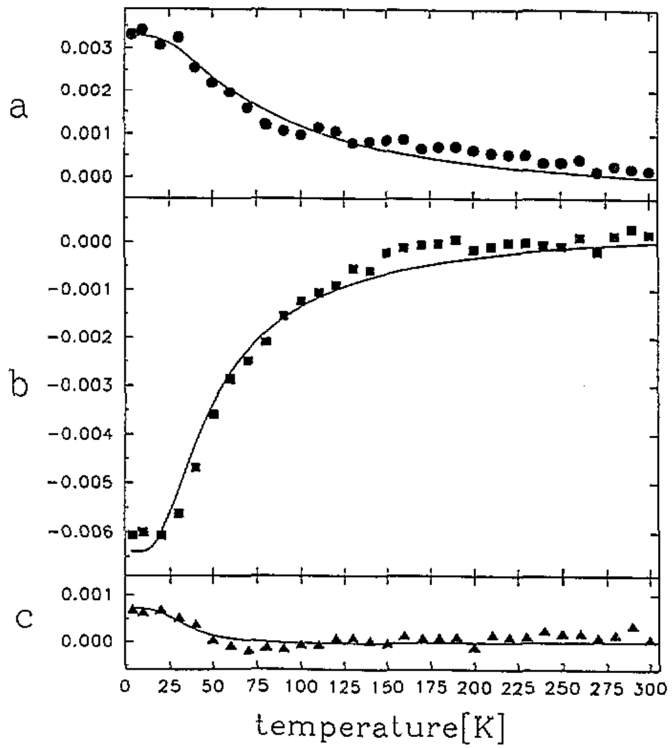

Figure 2. Experimentally determined differences of the normalized lattice parameters in the *a*, *b* and *c* directions of $TmCu_2$ and YCu_2 (symbols) together with the calculated results (curves).

Table 1. CF parameters for the orthorhombic $TmCu_2$ compound.

B_2^0	B_2^2	B_4^0	B_4^2	B_4^4
−0.94 K	−1.23 K	-0.9×10^{-2} K	-0.39×10^{-2} K	-0.36×10^{-2} K
B_6^0	B_6^2	B_6^4	B_6^6	
0.58×10^{-4} K	2.47×10^{-4} K	-0.48×10^{-4} K	6.31×10^{-4} K	

4. Summary

The anisotropic thermal expansion of $TmCu_2$ has been measured using x-ray powder diffraction. We were able to show that these anomalies in the anisotropic thermal expansion of $TmCu_2$ are due to the CF influence and can be described quantitatively, if we use the CF parameters published by Gubbens *et al* [2]. This analysis is based on the assumption that the elastic and magnetoelastic coupling parameters are temperature independent and can be determined by a fit to the experimental data. Recently we applied the same procedure for the analysis of the anisotropic thermal expansion of $ErCu_2$ and $NdCu_2$ [1] with the similar success.

Acknowledgments

This work was supported by the Austrian Science Foundation (FWF-Project P-8913).

References

[1] Gratz E, Rotter M, Lindbaum A, Mueller H, Bauer E and Kirchmayr H 1993 *J. Phys.: Condens. Matter* 5 567
[2] Gubbens P C M, Buschow K H J, Divis M, Heidelmann M and Loewenhaupt M 1992 *J. Magn. Magn. Mater.* **104–107** 1283