Determination of the critical exponent of the linear thermal expansion coefficient of nickel by neutron diffraction

1989 J. Phys.: Condens. Matter 1 5805

(http://iopscience.iop.org/0953-8984/1/33/026)

J. Phys.: Condens. Matter 1 (1989) 5805–5810. Printed in the UK

LETTER TO THE EDITOR

Determination of the critical exponent of the linear thermal expansion coefficient of nickel by neutron diffraction

T A Faisst†
Ludwig-Maximilians-Universität München, Sektion Physik, Schellingstr. 4, D-8000 München 40, Federal Republic of Germany

Received 16 June 1989

Abstract. The linear thermal expansion coefficient α has been measured on a nickel single crystal with a high-resolution neutron back-scattering diffractometer near the magnetic phase transition. From α, the critical part of the thermal expansion coefficient α_c was separated and fitted to a power-law equation $\alpha_c^{\pm} = A^{\pm} t^{-\mu^{\pm}} + B^{\pm}$ within the reduced temperature range $t = |(T - T_C)/T_C| = 10^{-2}$ to 10^{-3}. The critical exponent and the universal amplitude ratio are -0.09 and 1.3, respectively. These values are in good agreement with a measurement on polycrystalline nickel and with the values predicted by the renormalisation theory for the specific heat of a 3D Heisenberg model.

At the magnetic phase transition of nickel, the lattice expansion shows an anomaly on heating the crystal from the ferromagnetic to the paramagnetic state. This anomaly was investigated by a few authors on polycrystalline (Kollie 1977, Major *et al* 1971, Yousuf *et al* 1986) and on single-crystal (Söffge *et al* 1977) nickel samples. The results differ considerably from each other and two of them (Major *et al* 1971, Söffge *et al* 1977) did not take into account the non-critical contribution to the lattice expansion in their analysis. Therefore, no reliable values exist for the critical parameters derived from single crystals and it is necessary to take a new measurement to get more accurate data.

The neutron back-scattering technique was first developed by Alefeld (1966, 1968, 1969) at the Forschungsreaktor München (FRM)/Garching in the late sixties. Figure 1 shows the principles of the back-scattering method. The most important feature is the use of two single crystals with lattice planes that are parallel to each other and nearly perpendicular to the incident neutron beam. All neutrons that satisfy the Bragg equation are removed from the incident neutrons: the spectrum shows a dip at the corresponding wavelength behind the first crystal. This dip is analysed by a second crystal, which is moved sinusoidally against the first by a velocity drive, and the back-scattered intensity is stored as a function of the velocity in a multichannel analyser. A change Δa in the

† Present address: Mannesmann Demag AG, Carl-Legien-Str. 15 D-6050 Offenbach/Main, Federal Republic of Germany.

0953-8984/89/335805 + 06 $02.50

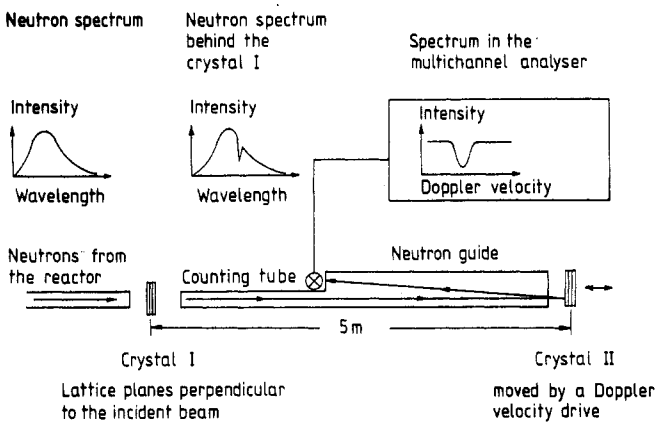

Figure 1. The principles of the neutron back-scattering diffractometer at the FRM (explanation in the text).

lattice constant a_{hkl} of the crystal I causes a shift Δv of the spectrum. The shift Δv is related to Δa by

$$\Delta a/a_{hkl} = \Delta v/v_{hkl}. \tag{1}$$

Here v_{hkl} describes the velocity of the neutrons that corresponds to the (hkl) reflection of crystal I.

If the lattice is changed by a temperature variation ΔT the coefficient of linear thermal expansion α can be determined by

$$\alpha = (\Delta a/a_{hkl})(1/\Delta T) = (\Delta v/v_{hkl})(1/\Delta T). \tag{2}$$

Figure 2 shows a typical line profile of the back-scattering diffractometer. The two spectra are recorded successively at different temperatures. It is seen from the diagram that a change in temperature causes a shift of the spectrum that is proportional to the change in the lattice constant.

More details of the back-scattering diffractometer are described by Alefeld (1968) and Faisst (1988).

Two nickel single crystals with dimensions of about 30 mm × 15 mm × 2.5 mm are used. Each crystal is cut by spark erosion and etched afterwards. It should be mentioned that a layer of about 1 mm was removed by the chemical process at each side of the crystal because the surfaces are destroyed within a depth of 1 mm by spark erosion (Faisst 1988). The crystals were not annealed because no change in the quality of the crystals could be observed at temperatures of about 800 °C. On the other hand, the crystals recrystallise at temperatures above 1100 °C and the onset of twinning occurs.

The linear thermal expansion coefficient α was calculated from the observed shift Δv of the spectrum using the relation (2). The critical contribution to the thermal expansion coefficient α_c is plotted in figure 3. This critical part is obtained by subtracting α_p (in K^{-1}) = $9.22 \times 10^{-9} T$ (in K) + 8.94×10^{-6} from the observed value α, i.e. $\alpha_c = \alpha - \alpha_p$. α_p is the paramagnetic non-critical contribution to the expansion near the critical point, extrapolated from measured data (Kollie 1977), obtained in the paramagnetic region of nickel far above T_C.

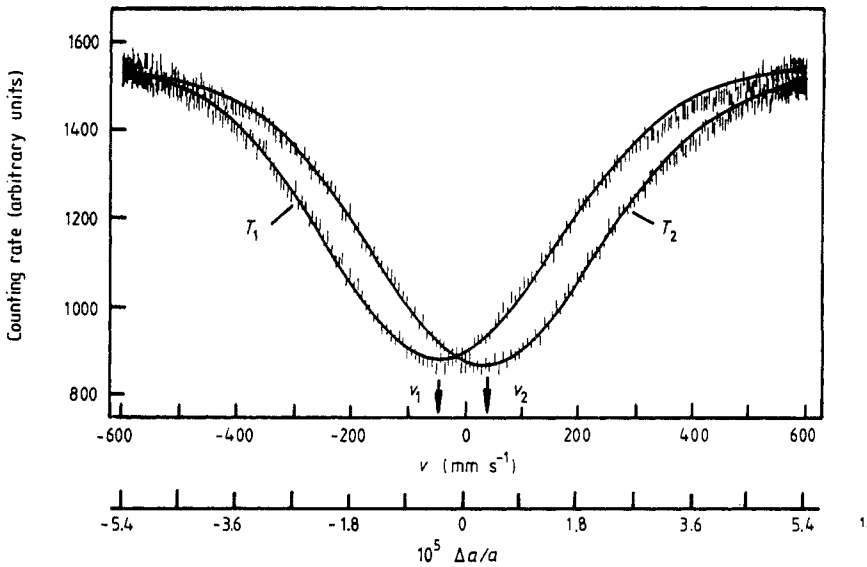

Figure 2. Typical line profile of the back-scattering diffractometer at two different temperatures. This profile corresponds to the (200) reflection. A least-squares fit of a Gaussian to the data is represented by the full curve. The vertical bars denote the statistical error of the counting rate. T_1 differs from T_2 by an amount of 4.28 K, which results in a shift $|v_1 - v_2|$ of 77.4 mm s^{-1}. The smallest shifts that can be measured are 0.5 mm s^{-1} or 5×10^{-7}. These values are valid for nickel single crystals and for 10 h of measurement time.

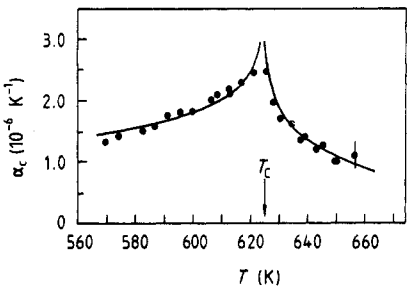

Figure 3. The critical part α_c of the thermal expansion coefficient of nickel near the Curie temperature T_C. The full curve is fitted to the data with a least-squares method using expression (3). The vertical bar denotes the whole error whose main contribution arises from the uncertain determination of the minimum of the spectrum.

The critical part of the linear thermal expansion α_c shown in figure 3 was fitted to an expression of the form

$$\alpha_C^{\pm} = A^{\pm} t^{-\mu^{\pm}} + B^{\pm} \tag{3}$$

where A, t, μ and B are the amplitude, the reduced temperature $(T - T_C)/T_C$ (where T_C is the Curie temperature), the critical exponent and a constant, respectively. The plus sign refers to above T_C, the minus sign to below T_C.

If the data were fitted above and below T_C separately, the predicted scaling law $\mu^- = \mu^+$ (Kadanoff *et al* 1967, Fisher 1974) and the requirement $B^- = B^+$ are not fulfilled (see table 1). This requirement is very important in analysing critical data because for negative exponents expression (3) describes a cusp-like behaviour with finite values for B^+ and B^- at T_C, which is the case for nickel. A difference in these values of the constants denotes a jump at the Curie temperature that should not appear at a continuous phase

Table 1. Values of the critical parameters of the power-law equation (3) obtained from a least-squares fit of the critical part of the linear thermal expansion coefficient carried out for various constraints used in our analysis. The value of the Curie temperature is also obtained by the fit. Its value is at the lower end of the temperature range determined by many of the experiments on nickel (Stierstadt *et al* 1984). The parameters are defined within ±5%.

Constraints used in the least-squares fit		T_C (K)	μ^-	μ^+	A^- ($10^{-6}K^{-1}$)	A^+ ($10^{-6}K^{-1}$)	A^+/A^-	B^- ($10^{-6}K^{-1}$)	B^+ ($10^{-6}K^{-1}$)
No constraints	$T < T_C$	625.15	−0.64		−5.50			2.70	
	$T > T_C$	625.0		−0.094		−7.20	1.31		6.40
Continuity at T_C, i.e. $B^- = B^+$	$T < T_C$	625.0[a]	−0.087		−5.90		1.22	6.40	
Scaling law, $\mu^+ = \mu^-$,	$T < T_C$	625.0[a]	−0.094		−5.50		1.31	6.00	

[a] T_C was held fixed during the fit procedure at the value obtained for $T > T_C$.

Table 2. The Curie temperature T_C, critical exponent μ, amplitudes A, universal amplitude ratio A^+/A^- and constants B^+, B^- of the critical part of the linear thermal expansion coefficient of nickel. The theoretical values given in the last line are calculated with a ε-expansion ($\varepsilon = 4 - d$) for the specific heat of a 3D Heisenberg model

Reference Sample Method of measurement	Kollie (1977) Polycrystal Dilatometer	Yousuf *et al* (1986) Polycrystal X-ray powder diffractometer	This work Single crystal Neutron back-scattering diffractometer	Theory
T_C (K)	628.3	629.325	625.0	
$\mu^- = \mu^+$	−0.093	−0.101	−0.094	−0.100[a]
A^- (10^{-6} K^{-1})	−6.87	not given	−5.50	
A^+ (10^{-6} K^{-1})	−7.91	not given	−7.20	
A^+/A^-	1.15	0.67	1.31	1.40[b], 1.24[c]
B^- (10^{-6} K^{-1})	6.87	not given	6.00	
B^+ (10^{-6} K^{-1})	6.73	not given	6.40	
$t = \lvert(T - T_C)\rvert/T_C(10^{-3})$ $T < T_C$	32–1.4	not given	87–4.5	
$t = \lvert(T - T_C)\rvert/T_C(10^{-3})$ $T > T_C$	26–0.8	not given	52–2.5	

[a] Fisher (1974).
[b] Brezin *et al* (1974), first order ε-expansion.
[c] Bervillier (1976), second order ε-expansion.

transition. Ahlers and Kornblit (1975) have pointed out in their reanalysis of specific heat data for different Heisenberg magnets that it is important to use the theoretically predicted constraint of equal critical exponents above and below T_C as well as the requirement that $B^- = B^+$ to obtain the best values for the parameters in a least-squares fit. If we carry out the least-squares fit with the above-mentioned constraints, the results are in good agreement with the theoretical predictions for a 3D Heisenberg model (see tables 1 and 2).

Here we should emphasise that no theoretical calculations exist for the critical exponent μ and the universal amplitude ratio A^+/A^- of the thermal expansion coefficient. Therefore, we take the usual assumption that the critical parameters of the heat capacity and of the thermal expansion coefficient describing the transition should be the same (Söffge *et al* 1977, Callen and Callen 1965).

In table 2, different measurements are compared with the theory. It can be seen that all three sets of authors have found nearly the same value for the critical exponent $\mu^- = \mu^+ \simeq -0.1$, which agrees well with the calculations by Fisher (1974). For the universal amplitude ratio A^+/A^-, we have obtained a value that is between the first- and second-order approximation in $\varepsilon(\varepsilon = 4 - d)$, where d is the dimension of the system). The value found by Kollie (1977) is about ten per cent smaller than our value but is still in the range covered by the theory, whereas the value given by Yousuf *et al* (1986) is too small. The comparison between our results and the results of Kollie (1977) shows that the absolute values of the amplitudes and the constants are in satisfactory agreement.

The investigation of the linear thermal expansion of nickel gives the same values of the ciritical exponent and the amplitude ratio as expected for the heat capacity by the renormalisation theory. The assumption of the same temperature behaviour of thermal expansion and specific heat near the critical point therefore seems justified. To obtain reasonable results, the fit procedure has to be carried out with the considerations of the

scaling law and the continuity of the transition for a negative exponent. All the critical parameters are close to those predicted by renormalisation theory for a 3D Heisenberg model.

I would like to thank Professor Dr K Stierstadt for a critical reading of this Letter. This work was supported by the Bundesministerium für Forschung und Technologie, Federal Republic of Germany.

References

Ahlers G and Kornblit A 1975 *Phys. Rev.* B **12** 1938
Alefeld B 1966 *Sitzungsber. Bay. Akad. Wiss. Math. Naturwiss. Kl.* **11** 109
—— 1968 *Dissertation* Technische Uniersität München
—— 1969 *Z. Phys.* **222** 155
Bervillier C 1976 *Phys. Rev.* B **14** 4964
Brezin E, Le Guillon J C and Zinn-Justin J 1974 *Phys. Lett.* **47A** 285
Callen E and Callen H B 1965 *Phys. Rev.* **139** A455
Faisst T 1988 *Dissertation* Ludwig-Maximilians-Universität München
Fisher M 1974 *Rev. Mod. Phys.* **46** 597
Kadanoff L P, Götze W, Hamblen D, Hecht R, Lewis E A S, Palciauskas V V, Payl M, Swift J, Aspnes J and Kane J 1967 *Rev. Mod. Phys.* **39** 395
Kollie T G 1977 *Phys. Rev.* B **16** 4872
Major J, Mezei F, Nagy E, Svab E and Tichy G 1971 *Phys. Lett.* **35A** 377
Söffge F, Steichele E and Stierstadt K 1977 *Phys. Status Solidi* a **42** 621
Stierstadt K, Anders R and von Hörsten W 1984 *Experimental Values of Critical Exponents and Amplitude Ratios at Magnetic Phase Transitions; Physics Data* **20–1** 79
Yousuf M, Sahu P Ch, Jajoo H K, Rajagopalan S and Govinda K 1986 *J. Phys. F: Met. Phys.* **16** 373