TEMPERATURE DEPENDENCE OF THE THERMAL EXPANSION COEFFICIENT, BULK MODULUS AND MAGNETIC GRUENEISEN CONSTANT OF NICKEL NEAR THE CURIE POINT

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TEMPERATURE DEPENDENCE OF THE THERMAL EXPANSION COEFFICIENT, BULK MODULUS AND MAGNETIC GRÜNEISEN CONSTANT OF NICKEL NEAR THE CURIE POINT

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Abstract. — Linear thermal expansion and bulk modulus are measured by the neutron backscattering technique in a nickel single crystal. The critical exponent of the thermal expansion coefficient agrees well with the theory of the specific heat for the Heisenberg model. The bulk modulus shows a small peak at the Curie point.

Although some measurements of the thermal expansion coefficient in the critical region of nickel [1-4], had been performed there are no reliable data for a single crystal. Moreover the results differ considerably from each other and some of the authors do not take the noncritical contribution into consideration in their analyse.

The neutron backscattering technique [5, 6] can be used to measure changes in the lattice constant. A new set-up [7] of the backscattering diffractometer at the Forschungsreaktor München is used to determine the linear thermal expansion coefficient and the bulk modulus of nickel near the Curie point. A resolution of about $1 \times 10^{-5}$ in lattice changes has been achieved. The crystals were grown by the method of Czochralski and have a purity of 99.999%.

To obtain the correct critical magnetic contribution of the linear thermal expansion coefficient $\alpha_{m}$ the non-critical part has to be subtracted from the measured expansion coefficient. The noncritical part, which is an extrapolation from the high temperature paramagnetic region to the region near the phase transition, was taken from the measurement of Kollie [3]. The critical contribution to the linear thermal expansion is plotted in figure 1a and the data were fitted to a power law (for explanation see Tab. I)

$$\alpha_{m} = \alpha^{\pm} T^{-\alpha^{\pm}} + B^{\pm}.$$  (1)

The data were fitted with the constraint $\alpha^{-} = \alpha^{+}$ to obey the scaling relation. Ahlers and Kornblit [11] pointed out that certain constraints are necessary to get reasonable results. The results are compared with theory [12] and with the measurements of Kollie [3] in table I. Good agreement is found although Kollie used a polycrystal.

The isothermal bulk modulus $B_{T}$ is defined as

$$B_{T} = -V \left( \frac{\partial p}{\partial V} \right)_{T}$$  (2)

($V$: volume, $p$: hydrostatic pressure). On the assumption, that nickel has a cubic symmetry below the Curie temperature, the bulk modulus can be expressed by

$$B_{T} = -\frac{1}{3} \left( \frac{\partial p}{\partial a} \right)_{T}$$  (3)

Table I. — Results of a least-squares fit of the magnetic part of the linear thermal expansion coefficient $\alpha_{m}$. The function used for the fit is a power law $\alpha_{m}^{\pm} = A^{\pm} t^{-\alpha^{\pm} + B^{\pm}}$ with the amplitude $A^{\pm}$, the reduced temperature $t = (T - T_{c})/T_{c}$, the Curie temperature $T_{c}$ and the constant $B^{\pm}$. The plus and minus signs refer to above and below $T_{c}$, respectively. The results are compared with the measurement of Kollie [3] and with theory.

<table>
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<th>Kollie</th>
<th>This work</th>
<th>Theory</th>
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<td>-0.094</td>
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<td>-5.5</td>
<td></td>
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<td>1.31</td>
<td>1.40 [9]</td>
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<tr>
<td>$10^{6} B^{-}$ [K$^{-1}$]</td>
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<td>6.0</td>
<td></td>
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<tr>
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<tr>
<td>$-8.0 \times 10^{-4}$</td>
<td>$-2.5 \times 10^{-3}$</td>
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</table>

with the lattice constant $a$. To determine the bulk modulus, the change of the lattice constant due to a hydrostatic pressure increase from 1 to 100 bar was measured. Figure 1b shows the bulk modulus in the vicinity of the phase transition. Although the relative uncertainties are large, $B_{T}$ is significantly larger below $T_{c}$ than above. Near the critical point the bulk modulus shows a cusp-like behavior in contrast to theoretical calculations [14] which predict a softening at the phase transition.

The pressure dependence of the Curie temperature can be expressed by

$$\frac{\partial T_{c}}{\partial p} = \gamma_{m} \frac{T_{c}}{B_{T}} = \frac{3 \alpha_{m} V^{(m)}}{C_{m}^{(m)}} . T_{c}$$  (4)

with the magnetic Grüneisen constant

$$\gamma_{m} = 3 \alpha_{m} V^{(m)} . B_{T}/C_{m}^{(m)}$$  [15]

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\( C_m^{(m)} \): molar magnetic specific heat; \( V^{(m)} \): molar volume. It should be emphasized that \( \frac{\partial T_c}{\partial p} \) do not depend on the bulk modulus as it can be seen from the second expression of equation (4).

Leger et al. [17] measured the shift of the Curie temperature with pressure and found the value 0.42 K/kbar. From figure 1 we have \( T_c \approx 625 \text{ K}, \alpha_m \approx 2.5 \times 10^{-5} \text{ K}^{-1} \) and \( B_T \approx 1.94 \times 10^{11} \text{ N/m}^2 \). With \( V^{(m)} = 6.8 \times 10^{-6} \text{ m}^3/\text{mol} \) and \( C_m^{(m)} \approx 9.5 \text{ J/(mol.K)} \) [16] we obtain the Grüneisen constant \( \gamma_m \approx 1.0 \) and the pressure dependence of \( \frac{\partial T_c}{\partial p} = 0.32 \text{ K/bar} \). This value is in satisfying agreement with the result of Leger et al.

**Fig. 1.** – (a) Magnetic contribution to the linear thermal expansion coefficient \( \alpha_m \) of nickel with a power law fit (solid line). (b) Isothermal bulk modulus \( B_T \) in the vicinity of the Curie point. The bars indicate the errors of the measured values.

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