

Magnetization of nickel in a field up to 320 kOe at temperatures up to 700 K

B. K. Ponomarev and V. G. Tissen

Institute of Solid-State Physics, USSR Academy of Sciences
(Submitted January 24, 1977)
Zh. Eksp. Teor. Fiz. 73, 332-341 (July 1977)

The magnetization of a polycrystalline specimen of nickel was measured in a pulsed magnetic field up to 320 kOe, over the temperature range from 283 to 693 K. It is shown that at temperatures from 550 to 700 K, the behavior of the magnetization of nickel is satisfactorily described by the equation of the band theory of ferromagnetism, when terms of the second order of smallness in the square of the magnetization and the square of the temperature are taken into account. From the results of the magnetization measurements, by use of the equations of the band theory of ferromagnetism, estimates are made of the exchange splitting and of the electronic specific-heat coefficient of nickel; they agree satisfactorily with the values in the literature.

PACS numbers: 75.30.Cr, 75.10.Lp, 75.40.-s, 75.50.Cc

It has been shown in many papers (see, for example, Refs. 1 and 2) that the ferromagnetism of nickel is intimately connected with its band structure. It therefore seems appropriate to investigate the possibility of describing the experimental temperature and field dependence of the magnetization of nickel by means of the relations of the theory of band ferromagnetism. The simplest magnetic equation of state of a band ferromagnet was obtained by Wohlfarth and Edwards^[3,4] for the case of very weak band ferromagnetism, by expansion of Stoner's equations^[5] as far as the second derivative of the density-of-states function with respect to energy. It is well known that the Wohlfarth-Edwards equation^[3,4] does not give a satisfactory description of the magnetic properties of nickel. The question arises whether this fact is a consequence of the inapplicability, in principle, of the Stoner-Wohlfarth procedure to the description of the magnetic properties of nickel, or a consequence of the fact that in the Wohlfarth-Edwards equation^[3,4] an insufficient number of terms was taken into account in the expansion of Stoner's equations.^[5]

A development of the Stoner-Wohlfarth theory was given in Ref. 6. The magnetic equation of state obtained in Ref. 6 can be written in the form

$$\begin{aligned} H/\sigma(H, T) = & a_{10} + a_{12}T^2 + a_{14}T^4 + a_{16}T^6 + \dots \\ & + a_{30}\sigma^2(H, T) + a_{32}\sigma^2(H, T)T^2 + a_{34}\sigma^2(H, T)T^4 + \dots \\ & + a_{50}\sigma^4(H, T) + a_{52}\sigma^4(H, T)T^2 + \dots + a_{70}\sigma^6(H, T) + \dots \end{aligned} \quad (1)$$

Here $\sigma(H, T)$ is the magnetization per unit mass as a function of the field H and the temperature T .

The conditions for applicability of an equation of the type (1) can be written as follows:

$$\delta_1 = (\mu_B \lambda \sigma(H, T) + \mu_B H) / \varepsilon_{F1} \ll 1, \quad (2)$$

$$\delta_2 = (\mu_B \lambda \sigma(H, T) + \mu_B H) / \varepsilon_{F2} \ll 1, \quad (3)$$

$$t_1 = kT / \varepsilon_{F1} \ll 1, \quad (4)$$

$$t_2 = kT / \varepsilon_{F2} \ll 1. \quad (5)$$

Here λ is the molecular-field constant, μ_B is the Bohr magneton, $\Delta(H, T) = 2\mu_B \lambda \sigma(H, T)$ is the exchange splitting, k is Boltzmann's constant, and $2\mu_B H$ is the Zeeman

splitting. The values of ε_{F1} and ε_{F2} , which represent, respectively, the widths of the filled and of the unfilled parts of the band in the paramagnetic state, were calculated theoretically for nickel in Ref. 7. The values obtained were $\varepsilon_{F1} = 4$ eV and $\varepsilon_{F2} \approx 0.3$ eV. There, also, was obtained the value of the exchange splitting in nickel at $T = 0$ K: $\Delta_0 = 0.37$ eV. By means of the relations (2)-(5) and the known values of ε_{F1} , ε_{F2} , and Δ_0 , one can estimate the limits of applicability of Eq. (1) if one knows the field and temperature dependence of the magnetization of the material under study. If in Eq. (1) one takes into account only the terms of lowest order in T^2 and σ^2 , one gets the Wohlfarth-Edwards equation^[3,4]

$$H/\sigma = a_{10} + a_{12}T^2 + a_{30}\sigma^2. \quad (6)$$

For comparison of Eq. (1) with experiment, the experimental data must permit an accurate separating out of the nonlinear contribution to the field dependence of the magnetization. The obtaining of such data requires measurements in a sufficiently strong magnetic field. In a number of papers^[8-10] the magnetization of nickel has been investigated in fields of order 10^5 Oe at two or three values of the temperature, from helium to room temperature. At these temperatures, the effect of the field on the magnetization of nickel is very small.

It has been shown^[11,12] that for investigation of the paraprocess, a temperature interval that contains the Curie point is most suitable. The magnetization of nickel at temperatures of the order of the Curie temperature has been investigated^[13] in a field up to 180 kOe. It was shown that at temperatures from 625 to 690 K, the function $H/\sigma = f(\sigma^2)$ is linear at sufficiently large values of the field.

We have measured the magnetization of a polycrystalline specimen of electrolytic nickel over the temperature interval from 283 to 693 K, in a pulsed magnetic field of intensity up to 320 kOe, with pulse duration 0.01 sec. The measurements were made by the induction method. In the measurement process, the curve that describes the field dependence of the magnetization

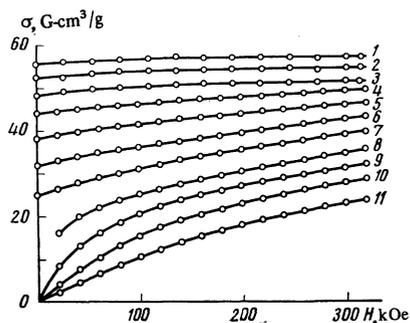


FIG. 1. Isotherms of the magnetization of nickel for various values of the temperature (in K): 1, 283.5; 2, 365; 3, 457; 4, 502; 5, 546; 6, 583; 7, 608; 8, 633; 9, 649; 10, 668; 11, 693.

is photographed from the oscillograph screen. The oscillograms are processed on a general-purpose measuring microscope UIM-21. The relative error of the magnetization measurements (spread of the experimental points on the field-dependence curves) does not exceed $\delta\sigma = \pm 0.5 \text{ G cm}^3/\text{g}$, which amounts to 1% of the maximum value of the magnetization of nickel. The relative error in the values of the magnetic field does not exceed $\delta H = \pm 3 \text{ kOe}$, which amounts to $\sim 1\%$ of the maximum value of the field. The magnetization scale was calibrated on the basis of the data of Crangle and Goodman.^[14] The absolute values of the field were determined by means of a test coil and an RC integrating circuit with an error of order 8%. The specimen has the form of a cylinder of length 10 mm and diameter 3 mm. The demagnetizing field at the maximum value of the magnetization amounts to $\sim 0.7 \text{ kOe}$, or 0.2% of the maximum value of the field. The demagnetizing field may be neglected, since it is less than the relative error of measurement of the magnetic field, $\delta H = 3 \text{ kOe}$. To decrease the effect of the eddy currents, the specimen was cut into four parts along two mutually perpendicular planes containing the axis of the cylinder. Under these conditions, the effect of the eddy currents on the value of the field inside the specimen does not exceed 0.1% of the value of the field outside the specimen.

The pulsed-field solenoid was immersed in liquid nitrogen. The working volume of the solenoid was hermetically isolated against penetration of liquid nitrogen into it. The specimen is heated with a furnace fed from a stabilized power supply B5-21. The specimen temperature establishes itself in the process of natural heat exchange between the operating volume and the dewar containing the liquid nitrogen. The oscillogram is taken when the drift of the specimen temperature does not exceed 0.1 K per minute. The temperature difference between the ends of a specimen of length 10 mm does not exceed 2 K at temperature 700 K and decreases with lowering of the temperature. The temperature is measured with a chromel-alumel thermocouple. The relative error of the temperature measurements is 2.5 K at $T = 700 \text{ K}$ and decreases with lowering of the temperature.

The process of magnetization of the specimen is al-

most adiabatic. The departure from adiabaticity does not exceed 15%. This estimate is obtained for a pulsed field of rectangular form. It can be shown that the departure from adiabaticity is less for field pulses of sinusoidal form than for a pulse of rectangular form.

The magnetocaloric effect was calculated by use of the relation

$$dT = \frac{T}{C_\sigma} \left(\frac{\partial H}{\partial T} \right)_\sigma d\sigma. \quad (7)$$

Here C_σ is the specific heat at constant magnetization. The experimental function $(\partial H / \partial T)_\sigma = f(\sigma)$ was obtained by constructing adiabatic lines of equal magnetization according to the experimental adiabatic curves of the magnetization. The value used in the calculation was $C_\sigma = 7 \text{ cal/g atom deg}$, independent of temperature. Neglect of the temperature dependence of the magnetization introduces into the calculation of the magnetocaloric effect an error of order 1 K. Calculation of the magnetocaloric effect was carried out by a method of successive approximations. The result of the second approximation differs from the result of the first approximation by less than 1 K. The magnetocaloric effect reaches 10 K near the Curie temperature at field 320 kOe and decreases with increasing distance from the Curie temperature. On the basis of the calculation of the magnetocaloric effect, isothermal lines of equal magnetization were obtained from the adiabatic lines of equal magnetization. The intersections of the isothermal lines of equal magnetization by the straight lines $T = \text{const}$ in the T, H plane give isotherms of the magnetization. Isotherms of the magnetization of nickel, obtained from experimental adiabatic curves of the magnetization after calculation of the magnetocaloric effect, are shown in Fig. 1. The increase of magnetization with field, over practically the whole range of field values investigated, occurs by the paraprocess. The nonlinearity of the paraprocess is clearly evident.

In the paramagnetic temperature range (Curves 9-11), the magnetization attains at 320 kOe about half the value of the spontaneous magnetization at absolute zero, $\sigma_0 = 58.58 \text{ G cm}^3/\text{g}$.^[14] From our measured values of the magnetization and from the literature data on ϵ_{F1} , ϵ_{F2} , and Δ_0 ,^[7] we found from relations (2)-(5), for various temperatures at field $H = 300 \text{ kOe}$, the values of δ_1 , δ_2 , t_1 , and t_2 given in Table I. The value of $\lambda \mu_B$ was found from the known values of Δ_0 and σ_0 at $T = 0 \text{ K}$. It is evident from the table that the values of δ_1 and t_1 are almost two orders of magnitude less than unity. It may be considered that conditions (2) and (4) are satisfied sufficiently well, for nickel, over the field and tem-

TABLE I. Values of δ_1 , δ_2 , t_1 , and t_2 for nickel from the relations (2)-(5), at various values of the temperature, in field $H = 300 \text{ kOe}$.

T, K	δ_1	δ_2	t_1	t_2	T, K	δ_1	δ_2	t_1	t_2
0	0.046	0.62	0.0000	0.000	693	0.018	0.25	0.0149	0.199
546	0.036	0.49	0.0118	0.157	1000	-	-	0.0216	0.288
608	0.031	0.42	0.0131	0.174	1500	-	-	0.0324	0.431
633	0.027	0.37	0.0136	0.181					

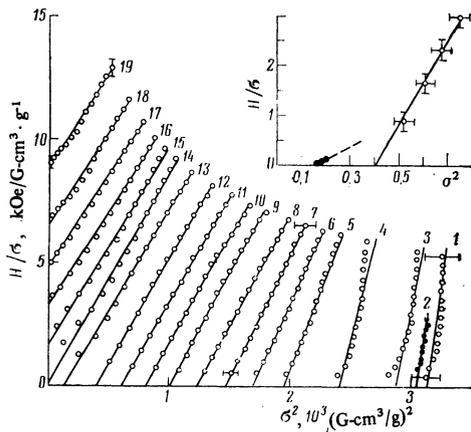


FIG. 2. Functions $H/\sigma = f(\sigma^2)$ for nickel at temperatures (in K): 1, 283; 2, 300; 3, 350; 4, 457; 5, 502; 6, 526; 7, 546; 8, 564; 9, 583; 10, 596; 11, 608; 12, 620; 13, 633; 14, 641; 15, 649; 16, 658; 17, 668; 18, 678; 19, 693. Curve 2 was plotted on the basis of the results of Ref. 10. The insert shows the function $H/\sigma = f(\sigma^2)$ at 619.5 K according to the data of Ref. 11 (dark points) and at 620 K according to our data (light points). The coordinate axes in the insert are stretched by a factor 2 as compared with Fig. 2.

perature range investigated. Conditions (3) and (5) are satisfied considerably worse. It may be supposed that this is the reason that the Wohlfarth-Edwards equation (6), which contains only terms of the first order of smallness in T^2 and σ^2 , disagrees with the experimental data for nickel. Allowance for terms of the next order of smallness in Eq. (1) leads to the equation

$$H/\sigma = a_{10} + a_{12}T^2 + a_{14}T^4 + a_{30}\sigma^2 + a_{32}\sigma^2T^2 + a_{30}\sigma^4. \quad (8)$$

If the Stoner-Wohlfarth treatment is correct, Eq. (8) should describe the magnetic properties of nickel better than the Wohlfarth-Edwards equation (6). It follows from the table that the agreement of theory with experiment, if it occurs at all within the temperature interval that we investigated (below 693 K), should be best in the high-temperature range. With lowering of the temperature, appreciable departures of theory from experiment are possible because of increase of the value of δ_2 . Figure 2 shows the experimental functions $H/\sigma = f(\sigma^2)$ found by us over the range of field values from 20 to 320 kOe. The dark points (Curve 2) are plotted from the results of Ref. 10. Within the limits of experimental error, the functions $H/\sigma = f(\sigma^2)$ for nickel are straight lines. Departures from linearity exceeding the experimental error are observed near the Curie temperature (Curves 13 and 14) in comparatively weak fields. This result agrees qualitatively with the results of Ref. 13.

In Ref. 11, the functions $H/\sigma = f(\sigma^2)$ for nickel were investigated at temperatures from 617 to 624.5 K, in a field up to 1.755 kOe. It was shown that over the range of field and temperature values investigated, these functions are linear. In the insert to Fig. 2 are plotted the functions $H/\sigma = f(\sigma^2)$ at temperature 619.5 K from Ref. 11 (dark points) and at temperature 620 K according to our data (light points). It is evident that with increase of field, the character of the function changes: in a field

up to 1.755 kOe (dark points), the slope is about three times smaller than in a field from 20 to 320 kOe (light points in the insert to Fig. 2, and Curve 12 in Fig. 2). The reasons for such a behavior of the functions $H/\sigma = f(\sigma^2)$ near the Curie temperature are unclear. Recognizing that over the greater part of the temperature range investigated no departures from linearity are observed, we consider our experimental functions $H/\sigma = f(\sigma^2)$ to be approximately linear. This assumption leads to a value of the Curie temperature that is somewhat too high as compared with the literature values. It is seen from Fig. 2 that the linear approximation in this case gives for the Curie temperature a value ~ 640 K. In Ref. 14 the value obtained was $T_c = 631$ K.

It is evident from Eq. (8) that the linear approximation to the functions $H/\sigma = f(\sigma^2)$ is equivalent to the case $a_{50} = 0$. The slope of the straight lines $H/\sigma = f(\sigma^2)$ in Fig. 2 depends on the temperature: it increases with lowering of the temperature. The temperature dependence of the slope, $B(T^2)$, can be obtained from Eq. (8) by differentiation with respect to σ^2 at constant temperature:

$$B(T^2) = \left[\frac{\partial (H/\sigma)}{\partial (\sigma^2)} \right]_T = a_{30} + a_{32}T^2. \quad (9)$$

Here it is assumed that $a_{50} = 0$. From (9) and the experimental relation $B(T^2)$, one can find the values of the coefficients a_{30} and a_{32} . The experimental relation $B(T^2)$ is shown in Fig. 3. For values of T^2 from $5 \cdot 10^5$ to $3 \cdot 10^5$ K² ($T \approx 700$ to 550 K), the value of B varies practically linearly with the square of the temperature, in accordance with (9). For $T^2 < 3 \cdot 10^5$ K² ($T < 550$ K) there is a noticeable departure of the $B(T^2)$ relation from linearity; this may be attributed to an increase of δ_2 with lowering of the temperature (see the table) and consequent weakening of the inequality (3). To describe the $B(T^2)$ relation for $T < 550$ K, it is apparently necessary to allow for terms of higher order in T^2 and σ^2 than is done in (8) and (9). By drawing a straight line through the experimental $B(T^2)$ points in the range $T^2 \approx (5 \cdot 10^5$ to $3 \cdot 10^5)$ K² ($T \approx 700$ to 550 K), we found the coefficient values $a_{30} = (13.1 \pm 1.0)$ Oe/(G cm³/g)³ and $a_{32} = -(1.23 \pm 0.30) \cdot 10^{-5}$ Oe/(G cm³/g)³ K² from the relation (9).

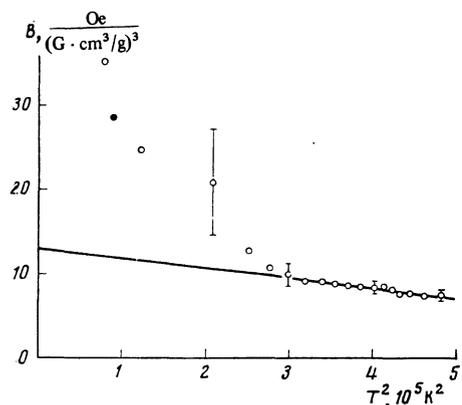


FIG. 3. Slope of the straight lines $H/\sigma = f(\sigma^2)$ (Fig. 2) as a function of the square of the temperature, $B(T^2)$. The dark point is the result of Ref. 10.

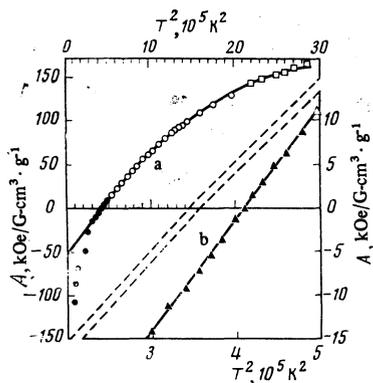


FIG. 4. Initial ordinate of the straight lines $H/\sigma=f(\sigma^2)$ (Fig. 2) as a function of the square of the temperature, $A(T^2)$. The coordinate axes in Fig. 4b are stretched by a factor ten as compared with Fig. 4a. ● and ▲, our results; ○ and △, results of Ref. 15; □, Ref. 16.

It follows from (8) that for the case under consideration, in which $a_{50}=0$, the value of

$$A(T^2)=a_{10}+a_{12}T^2+a_{14}T^4 \quad (10)$$

can be found by extrapolation of the experimental straight lines $H/\sigma=f(\sigma^2)$ plotted in Fig. 2 to their intersection with the H/σ axis. The value of $A(T^2)$ is the intercept that the straight line $H/\sigma=f(\sigma^2)$ at the corresponding temperature cuts off on the H/σ axis. It can be shown from (8) that the temperature function $A(T^2)$ intersects the temperature axis at the Curie point and that at temperatures above the Curie point, it has the physical meaning of inverse initial susceptibility. From the experimental temperature dependence of the value of $A(T^2)$, the coefficients a_{10} , a_{12} , and a_{14} can be found. Figure 4 shows the function $A(T^2)$ for nickel. The dark points were obtained from the results of our measurements by the method indicated above. The light points are the results of susceptibility measurements from Refs. 15 and 16. From the intersection of the $A(T^2)$ relation with the T^2 axis, the value of the Curie temperature was found to be $T_c \approx 640$ K.

From Fig. 4b it is seen that within the temperature interval $T^2 \approx (3 \cdot 10^5 \text{ to } 5 \cdot 10^5) \text{ K}^2$ ($T \approx 550 \text{ to } 700$ K), the $A(T^2)$ relation is, to within good accuracy, a straight line. For $T^2 < 3 \cdot 10^5 \text{ K}^2$ ($T < 550$ K), there is a noticeable departure from a straight line (Fig. 4a); this may be attributed to an increase of δ_2 with lowering of the temperature (see the table) and consequent weakening of the inequality (3). To describe the $A(T^2)$ relation for $T < 550$ K, it is necessary to allow for terms of higher orders in T^2 and σ^2 . At high temperatures (Fig. 4a), there is a departure from linearity because of increase of the contribution of the term $a_{14}T^4$ to the value of $A(T^2)$. By approximating the experimental function $A(T^2)$ by the relation (10) by the method of least squares over the temperature interval $T^2 = 3 \cdot 10^5 \text{ K}^2$ to $30 \cdot 10^5 \text{ K}^2$ ($T = 550 \text{ to } 1700$ K) (the curve in Fig. 4a), we found the coefficient values

$$a_{10} = -(5.14 \pm 0.20) \cdot 10^4 \text{ Oe}/(\text{G cm}^3/\text{g}),$$

$$a_{12} = + (0.136 \pm 0.010) \text{ Oe}/(\text{G cm}^3/\text{g})\text{K}^2,$$

$$a_{14} = - (2.15 \pm 0.45) \cdot 10^{-8} \text{ Oe}/(\text{G cm}^3/\text{g})\text{K}^4.$$

In order to estimate how sensitive the results of our calculations are to the value of the coefficient a_{14} , we set $a_{14}=0$ and found the values of the coefficients a_{10} and a_{12} by the linear approximation to the function $A(T^2)$ over the interval $T^2 = 3 \cdot 10^5$ to $5 \cdot 10^5 \text{ K}^2$ ($T = 550$ to 700 K) (the straight line in Fig. 4b). The differences in the values of the coefficients a_{10} and a_{12} for these two cases do not exceed 4%. The resulting changes of the parameters of the density-of-states curve and of the exchange splitting are also small. The analysis of the relations $B(T^2)$ (Fig. 3) and $A(T^2)$ (Fig. 4) shows that over the temperature interval (550 to 700) K in a field up to 320 kOe, the behavior of the magnetization of nickel can be described by Eq. (8).

At temperatures below 550 K, there are deviations from Eq. (8). We shall estimate these deviations. From (8) with $a_{50}=0$, we get for the spontaneous magnetization σ_0 at absolute zero

$$\sigma_0 = (-a_{10}/a_{30})^{1/3}. \quad (11)$$

Using the values we have found for the coefficients a_{10} and a_{30} , we get $\sigma_0 = 62.6 \text{ G cm}^3/\text{g}$, which exceeds by only 7% the experimental value $\sigma_0 = 58.58 \text{ G cm}^3/\text{g}$.^[14]

For the initial susceptibility χ_0 at absolute zero, we get from Eq. (8) on the supposition that $a_{50}=0$.

$$\chi_0 = -1/2a_{10}. \quad (12)$$

Hence for nickel $\chi_0 = 0.97 \cdot 10^{-5} \text{ cm}^3/\text{g}$. The susceptibility of nickel at $T = 4.2$ K has been found experimentally.^[9,10] In Ref. 10 the value found for the susceptibility, averaged over the interval of field values from 50 to 150 kOe, was $\chi(4.2 \text{ K}) = 0.19 \cdot 10^{-5} \text{ cm}^3/\text{g}$. In Ref. 9 the value obtained by averaging over the interval from 15 to 50 kOe was $\chi(4.2 \text{ K}) = 0.64 \cdot 10^{-5} \text{ cm}^3/\text{g}$. It was remarked^[10] that the susceptibility of nickel at 4.2 K decreases with increase of field. Hence it follows that the experimental value of the initial susceptibility of the paraprocess of nickel at 4.2 K must be larger than $0.64 \cdot 10^{-5} \text{ cm}^3/\text{g}$. Thus our estimate of the initial susceptibility of the paraprocess of nickel near 0 K agrees in order of magnitude with experiment. Relations have been obtained^[6] that relate the coefficients in equation (8) to the exchange-interaction parameter J , the value of the density of states of the magnetically active electrons at the Fermi level in the paramagnetic state, ν_F , and the values of the derivatives of the density-of-states function at the Fermi level in the paramagnetic state, ν'_F , ν''_F , ν'''_F , and ν''''_F . By use of these relations and of the coefficients in Eq. (8) found by us, we have found

$$J = 0.5 \text{ eV},$$

$$\nu_F = 4.54 \text{ states/atom eV},$$

$$\nu'_F = \pm 9.60 \text{ states/atom eV}^2,$$

$$\nu''_F = -1.06 \cdot 10^2 \text{ states/atom eV}^3,$$

$$\begin{aligned} \nu_F''' &= \mp 2.84 \cdot 10^3 \text{ states/atom eV}^4, \\ \nu_F'''' &= -6.15 \cdot 10^3 \text{ states/atom eV}^5. \end{aligned} \quad (13)$$

From the value of the exchange-interaction parameter J , we found the value of the exchange splitting in nickel at absolute zero:

$$\Delta_0 = 2\mu_B \lambda \sigma_0 = J\sigma_0 / N\mu_B = 0.33 \text{ eV}. \quad (14)$$

Here N is the number of atoms of nickel in unit mass, and $\sigma_0 = 62.6 \text{ G cm}^3/\text{g}$ is the calculated value of the spontaneous magnetization at $T = 0 \text{ K}$.

The estimate (14) agrees well with the result obtained in Ref. 7, $\Delta_0 = 0.37 \text{ eV}$. Values of the exchange splitting in nickel have also been calculated in other papers.^[17-21] The results for Δ_0 obtained in these papers lie in the interval from 0.2 to 0.8 eV, which agrees with our result in order of magnitude. Our value of the density of states at the Fermi level of paramagnetic nickel, $\nu_F = (4.54 \pm 0.37) \text{ states/atom eV}$, agrees well with the value $\nu_F = 4.2 \text{ states/atom eV}$.^[17]

The system of equations from Ref. 6, which we used to find the values of ν_F , ν_F' , ν_F'' , and ν_F''' , does not permit an unambiguous determination of the first and third derivatives of the density-of-states function: these values are determined except for sign, and the sign of the first derivative is always opposite to the sign of the third derivative. From the values we obtained for ν_F , ν_F' , etc., we calculated the density-of-states function of paramagnetic nickel near the Fermi level with fourth-derivative accuracy. The result of the calculation, for the values $\nu_F' = +9.6 \text{ states/atom eV}^2$ and $\nu_F''' = -2.84 \cdot 10^3 \text{ states/atom eV}^4$, is shown in Fig. 5. The width of the unfilled part of the band is $\epsilon_{F2} = 0.2 \text{ eV}$, which agrees satisfactorily with the data of Ref. 7. In view of the approximate nature of our calculations, one should not expect a detailed agreement of the form of our curve for the density of states with the results of the calculations of other authors.

The density-of-states curve corresponding to the second pair of values of ν_F' and ν_F''' is obtained from the curve of Fig. 5 by a mirror reflection with respect to the dotted line. This curve gives a total number of $3d$ and $3s$ electrons in nickel that is too low by orders of magnitude; it was therefore not considered. From the known values (13) of the parameters of the density-of-states curve and (14) of the exchange splitting, one can find the value of the density of states at the Fermi level for ferromagnetic nickel, ν_{FF} , by means of the relation

$$\nu_{FF} = \nu_F \left\{ 1 - \frac{\Delta_0^2}{8} \left[\left(\frac{\nu_F'}{\nu_F} \right)^2 - \frac{\nu_F'''}{\nu_F} \right] \right\}. \quad (15)$$

Calculation by formula (15) gives $\nu_{FF} = 2.85 \text{ states/atom eV}$. The corresponding value for the coefficient of electronic specific heat, $\gamma = (16.0 \pm 2.0) \cdot 10^{-4} \text{ cal/mol K}^2$, agrees well with the experimental result $\gamma = 17.4 \cdot 10^{-4} \text{ cal/mol K}^2$.^[19]

An estimate analogous to (15) can be made with fourth-derivative accuracy. This estimate gives $\gamma = 18.8 \cdot 10^{-4} \text{ cal/mol K}^2$. The corresponding formula is somewhat

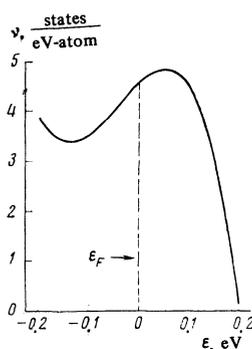


FIG. 5. Density-of-state curve of paramagnetic nickel, calculated from results of magnetization measurements in a strong field by use of the equations of the theory of band ferromagnetism.

cumbersome, and we shall not give it. It is clear from this that, despite the large discrepancies between theory and experiment in the determination of the low-temperature values of $B(T^2)$ (Fig. 3) and $A(T^2)$ (Fig. 4), the theory gives acceptable results for σ_0 , χ_0 , and γ .

Thus there is a basis for supposing that the relations of the Stoner-Wohlfarth theory of band ferromagnetism are in principle applicable to the description of the magnetic properties of nickel when account is taken of a sufficient number of terms in an equation of the type (1). It may be assumed that taking account of terms $a_{16}T^6$, $a_{34}\sigma^2T^4$, $a_{52}\sigma^4T^2$, $a_{70}\sigma^6$, etc., which we neglected when we analyzed the experimental results by use of (8), will give better agreement of the band theory with experiment. In order to determine the coefficients in these terms experimentally, it is necessary to increase the accuracy of the measurements considerably.

It should be mentioned that even when account is taken of terms of high order in T^2 and σ^2 , a discrepancy must occur between an equation of the type (1) and low-temperature experimental results for nickel, since this equation does not allow for effects due to spin waves. For more correct description of the magnetic properties of nickel at low temperatures, one needs equations combining the ideas of the theory of band magnetism and of spin-wave theory. Indications of this are contained in a number of papers^[22,23] in which it is shown that the temperature dependence of nickel at helium temperatures contains both spin-wave and Stoner terms. Furthermore, it should be mentioned that in Eq. (1) account has been taken only of the spin contribution to the magnetization; the contribution of the orbital motion of the electrons is ignored. Approximate description of the magnetic properties of nickel by use of this equation is possible because the orbital contribution to the magnetization of nickel is comparatively small (the value of the magnetomechanical ratio for nickel is close to two). Refinement of the theory obviously requires taking the orbital contribution into account.

¹D. C. Tsui, Phys. Rev. 164, 669 (1967).

²P. Goy and C. C. Grimes, Phys. Rev. B7, 299 (1973).

³E. P. Wohlfarth, J. Appl. Phys. 39, 1061 (1968).

⁴D. M. Edwards and E. P. Wohlfarth, Proc. Roy. Soc. Lond. A303, 127 (1968).

⁵E. C. Stoner, Proc. Roy. Soc. Lond. A165, 372 (1938).

⁶M. J. Besnus, Y. Gottehrer, and G. Munsch, Phys. Status

- Solidi (b) **49**, 597 (1972).
- ⁷L. Hodges, H. Ehrenreich, and N. D. Lang, *Phys. Rev.* **152**, 505 (1966).
- ⁸P. Kapitza, *Proc. Roy. Soc. Lond.* **A131**, 243 (1931).
- ⁹C. Herring, R. M. Bozorth, A. E. Clark, and T. R. McGuire, *J. Appl. Phys.* **37**, 1340 (1966).
- ¹⁰S. Foner, A. J. Freeman, N. A. Blum, R. B. Frankel, E. J. McNiff, Jr., and H. C. Praddaude, *Phys. Rev.* **181**, 863 (1969).
- ¹¹K. P. Belov and A. N. Goryaga, *Fiz. Met. Metalloved.* **2**, 3 (1956) [*Phys. Met. Metallogr.* **2**, No. 1, 1 (1956)].
- ¹²K. P. Belov, *Magnitnye prevrashcheniya (Magnetic Transitions)*, Fizmatgiz, 1959 (translation, Consultants Bureau, New York, 1961).
- ¹³S. Hatta, M. Matsui, and S. Chikazumi, *Int. Conf. Magnetism, Amsterdam*, abstracts, 1976, p. 136; *Proceedings (reprinted from Physica 86-88 B+C, Part I)*, p. 309.
- ¹⁴J. Crangle and G. M. Goodman, *Proc. Roy. Soc. Lond.* **A321**, 477 (1971).
- ¹⁵W. Sucksmith and R. R. Pearce, *Proc. Roy. Soc. Lond.* **A167**, 189 (1938).
- ¹⁶Y. Nakagawa, *J. Phys. Soc. Jap.* **11**, 855 (1956).
- ¹⁷S. Wakoh and J. Yamashita, *J. Phys. Soc. Jap.* **19**, 1342 (1964).
- ¹⁸C. S. Wang and J. Callaway, *Phys. Rev.* **B9**, 4897 (1974).
- ¹⁹M. Shimizu, T. Takahashi, and A. Katsuki, *J. Phys. Soc. Jap.* **18**, 801 (1963).
- ²⁰E. D. Thompson, E. P. Wohlfarth, and A. C. Bryan, *Proc. Phys. Soc. Lond.* **83**, 59 (1964).
- ²¹E. I. Zornberg, *Phys. Rev.* **B1**, 244 (1970).
- ²²M. S. Legkostupov, *Zh. Eksp. Teor. Fiz.* **61**, 262 (1971) [*Sov. Phys. JETP* **34**, 136 (1972)].
- ²³A. T. Aldred, *Phys. Rev.* **B11**, 2597 (1975).

Translated by W. F. Brown, Jr.

Density of electron levels in ferroelectric semiconductors

V. A. Malomed and V. L. Shneerson

Institute of Applied Physics Problems of the Belorussian State University
(Submitted February 10, 1977)
Zh. Eksp. Teor. Fiz. **73**, 342-347 (July 1977)

We consider the effect of the electron-phonon interaction on the electron density of states $g(\epsilon)$ in polarized semiconductors with soft optical phonons. It is shown that for weakly doped semiconductors the value of g depends strongly on ϵ near the Fermi surface and has a minimum on this surface. $g(0)$ becomes anomalously small near the ferroelectric transition point.

PACS numbers: 71.20.+c, 71.38.+i

INTRODUCTION

The spectra of the lattice vibrations of certain polar degenerate semiconductors contain soft (temperature-dependent) phonons. In the long-wave region, the spectrum of such soft transverse optical phonons is determined by the relation $\omega_i^2(\mathbf{q}) = \omega_0^2 + s\mathbf{q}^2$, where ω_0 is an anomalously small gap ($\omega_0 \ll \omega_D$), and the dispersion s is of normal order of magnitude.

The electron-phonon-interaction singularities typical of this situation were discussed in detail by one of us.^[1] The polarization part of the interaction is described, as usual, by a Fröhlich Hamiltonian. The transverse degrees of freedom make no contribution to the macroscopic polarization field. The corresponding deformation potential is usually small in comparison with the polarization potential. In the case of small ω_0 however, it is precisely the deformation contribution to the electron scattering by the lattice which is fundamental. In this paper we investigate the influence of this interaction on the electron level density $g(\epsilon)$ of a degenerate weakly doped semiconductor for states near the Fermi surface.

2. CORRECTIONS TO THE VERTEX FUNCTION

The effective electron-electron interaction, which includes exchange of soft phonons at $T=0$, is given by^[1]

$$D_0(\mathbf{q}, \omega) = \frac{4\pi e^2}{K^2} |C|^2 \frac{\epsilon_0(\mathbf{q}) \omega_i^2(\mathbf{q})}{\omega^2 - \omega_i^2(\mathbf{q}) + i\delta}, \quad (1)$$

where $\epsilon_0(\mathbf{q})$ is the static part of the dielectric constant of the lattice, and K is the reciprocal-lattice vector. The constant $|C| < 1$ is connected with the amplitude modulation of the Bloch functions. Using the Lyddane-Sachs-Teller relation for the long-wave region,^[1] we represent the interaction (1) in the form

$$D_0(\mathbf{q}, \omega) = 4\pi^2 \bar{a} s / [\omega^2 - \omega_i^2(\mathbf{q}) + i\delta], \quad (2)$$

where we have introduced the dimensionless electron-phonon coupling constant

$$\bar{a} = e^2 |C|^2 \epsilon_\infty \omega_i^2 / \pi s K^2, \quad (3)$$

ϵ_∞ is the dielectric constant due to the polarizability of the bound electrons, and ω_i is the frequency of the longitudinal optical phonons.

Let us examine the correction that must be introduced into the electron vertex function \mathcal{V} as a result of the interaction (2) at $T=0$. The corresponding diagram is shown in Fig. 1. The electron line corresponds here to the zero-order Green's function

$$G_0(\epsilon, \mathbf{p}) = [\epsilon - \mathbf{p}^2/2m + i\delta \operatorname{sign}(|\mathbf{p}| - p_0)]^{-1}.$$