Specific Heat of a Ferromagnetic Substance Above the Curie Point

C. DoMB AND M. F. SYKEs Wheatstone Laboratory, King's College, London, England (Received August 23, 1957)

High-temperature expansions for the specific heat of the Ising model are compared for the triangular and f.c.c. lattices. It is concluded that the "tail" of the specific heat curve above the Curie point is much smaller for the f.c.c. lattice, but is steeper in the immediate neighborhood of the Curie point. For the Heisenberg model for the f.c.c. lattice the tail is larger but apparently much less steep.

IN the absence of an exact solution of the three dimensional Ising model, the best source of information on the physical properties of the model would seem to be exact series expansions for the partition function at low and high temperatures. From the latter it is possible to derive a series expansion for the specific heat in inverse powers of the temperature, all the terms in the expansion being positive. Thus the behavior of the specific heat above the Curie point is determined by the asymptotic form of the coefficients in this series. To obtain reliable information regarding the nature of the specific heat anomaly, care must be taken to evaluate the coefficients correctly, and the position of the Curie point must first be estimated with considerable accuracy. Comparison with corresponding expansions for two-dimensional models for which exact solutions are available can also be most helpful.

Wakefield¹ derived several terms of the expansion for the simple cubic lattice, and although we have recently discovered small errors in the last two terms,² they are not large enough to affect his conclusions. However, it seemed to us that close-packed lattices, for which both odd and even terms occur in the expansion, could provide more information on the nature of the specific heat anomaly. Terms have been calculated up to $1/T⁹$ for the f.c.c. lattice, and are as follows:

 $C_v/R = 6K^2+48K^3+390K^4+3200K^5$ $+26584K^{6}+226374.4K^{7}+1971090.6K^{8}$ $+17428723.2K^9$. (1)

Here $K = J/kT$, and $-J$ is the energy of a pair of parallel spins. The corresponding series for the triangular lattice in two dimensions is

$$
C_v/R = 3K^2 + 12K^3 + 33K^4 + 80K^5 + 212K^6
$$

+ 649.6K⁷+2076.467K⁸+6652.953K⁹. (2)

For the triangular lattice an exact solution is available and the Curie point is known exactly $(kT_c/6J=0.606826)$. For the f.c.c. lattice, analysis of high-temperature susceptibility expansions has yielded an estimate' $kT_c/12J=0.816$, and this should be within 1% of the true value. To compare the specific heat curves for the two lattices, we express the expansions (1) and (2) in terms of the reduced variable $\kappa = T_c/T$, and we find for the f.c.c. lattice,

$$
C_v/R = 0.06257\kappa^2(1+0.8169\kappa+0.6778\kappa^2+0.5680\kappa^3+0.4818\kappa^4+0.4190\kappa^5+0.3725\kappa^6+0.3364\kappa^7),
$$
 (3)

and for the triangular lattice,

$$
C_v/R = 0.2263\kappa^2(1+1.0986\kappa+0.8298\kappa^2+0.5525\kappa^3+0.4021\kappa^4+0.3384\kappa^5+0.2971\kappa^6+0.2614\kappa^7). (4)
$$

In comparing (3) and (4) , we may say roughly that the term outside the parentheses represents the magnitude of the "tail" of the specific heat curve, and the term inside the parentheses represents the shape of the curve, particularly near the Curie point. It will be seen that the magnitude of the tail is much smaller for the f.c.c. lattice; this has already been noted by comparing the values of the entropy at the Curie point.⁴ But it will also be seen that the coefficients decrease less rapidly for the f.c.c. lattice and the specific heat curve is therefore sharper (and is thus certainly infinite). The extent of this sharpness can be analyzed by writing the ratio of successive coefficients a_{n+1}/a_n in (3) and (4) in the form $1+g/n$, and determining the value of $h(= g+1)$. A limiting constant value of h would correspond to $C_v/R \sim (1-\kappa)^{-h}$ (h=0 corresponding to a logarithmic singularity). Table I gives values of $h(=g+1)$ for successive terms for the two lattices. The values of h for the triangular lattice are much less regular than for the f.c.c. lattice, and we know from the exact solution that they will ultimately settle down to a value of $h=0$. The values for the f.c.c. lattice

TABLE I. Parameter $h=1-n+n a_{n+1}/a_n$ for successive terms in the expansions of Eqs. (3) and (4).

n	$h(\Delta$ lattice)	h(f.c.c.)
	1.0986	0.8169
	0.5106	0.6594
	-0.0025	0.5140
4	-0.0889	0.3930
	0.2079	0.3483
	0.2678	0.3341
	0.1589	0.3215

4 C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) 235, 247 (1956).

¹ A. J. Wakefield, Proc. Cambridge Phil. Soc. 47, 799 (1951).
² C. Domb and M. F. Sykes, Phil. Mag. 2, 733 (1957).
³ C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) 240, 214

^{(1957).}

decrease steadily, and seem to correspond to a singularity less steep than $(1-\kappa)^{-1}$.

It is interesting to look at the corresponding expansions for the f.c.c. lattice for the Heisenberg model. Fewer terms are here available, and corresponding to (1) we now have

$$
C_v/R = 18K^2 + 108K^3 + 90K^4 - 840K^5 + 6750K^6. \quad (5)
$$

The Curie point can be estimated from high-temperature susceptibility data as given³ by $kT_c/12J=0.695$. The reduced specific heat expansion corresponding to (3) is now

$$
C_v/R = 0.2588\kappa^2(1+0.7194\kappa+0.07188\kappa^2)
$$

 $-0.08044\kappa^3+0.07750\kappa^4$. (6)

It will be seen from the term outside the parentheses that the tail is considerably larger than for the Ising model. However the terms inside the parentheses do not show steady behavior, are much smaller, and are not all of the same sign. They seem to be consistent with a much less steep behavior near the Curie point, and possibly a finite value at the Curie point.

PHYSICAL REVIEW VOLUME 108, NUMBER 6 DECEMBER 15, 1957

Conductivity Mobilities of Electrons and Holes in Heavily Doped Silicon

GERHARD BACKENSTOSS Bell Telephone Laboratories, Murray Hill, New Jersey (Received August 8, 1957)

Electron and hole mobilities in silicon have been determined in a region in which ionized impurity scattering is predominant. Resistivities were measured by a four-point probe and impurity concentrations were obtained with radioactive tracers or from thermal neutron activation analysis. Measurements were taken with several Group III and Group V impurities up to concentrations of 6×10^{19} (cm⁻³) and 6×10^{18} $(cm⁻³)$ for *n*- and *p*-type silicon, respectively. The conductivity mobility can be calculated from these data by considering the percentage of ionized impurities. The electron mobility approaches 80 cm²/v-sec and the hole mobility 60 cm²/v-sec for the highest impurity concentrations. The comparison with measured Hall mobilities leads to a ratio μ_H/μ_c which agrees with theory. A comparison with the existing theory of impurity scattering yields better agreement for n -type silicon than for p -type. In the latter the measured mobilities are considerably smaller than the theoretical values.

INTRODUCTION

RIFT mobilities in semiconductors have been theoretically calculated by several authors. Values of the drift mobility in the higher concentration range can be obtained from the theories of impurity scattering by Conwell-Weisskopf¹ and Brooks-Herring.² In addition to this, several independent theoretical treatments of the ratio of Hall mobility to drift mobility for nondegenerate semiconductors are available.³⁻⁵ All treatments yield a ratio greater than unity. In the degenerate case this ratio approaches unity since the averaging of τ over energy becomes unimportant.

Various measurements of Hall mobilities are published for *n*- and p -type silicon.⁶⁻⁸ They cover a wide range of impurity concentrations and are generally in agreement.

Drift or conductivity mobilities have been measured Drift or conductivity mobilities have been measured
by Prince,⁹ Cronemeyer,¹⁰ and Horn.¹¹ Only the data

of Horn include the high-concentration range above 10^{17} (cm⁻³), but they are restricted to boron-doped silicon. His mobilities are higher than the reported Hall mobilities but smaller than theoretical mobilities. However, according to Carlson⁸ the reliability of the chemical calibration involved in this method appears to be doubtful. Carlson applies a correction which leads to lower mobilities.

The present investigation gives additional data for conductivity mobilities in the higher concentration range. Radioactive tracers or thermal neutron activation analysis have been used to determine impurity concentrations. This method was applied to several donor and acceptor elements.

METHOD

In heavily doped silicon the contribution of the minority carriers to the conductivity is negligible. Therefore, the conductivity mobility μ is obtained from the resistivity ρ by the relation

$$
\mu = 1/q\rho n, \tag{1}
$$

where *n* is the charge carrier density and q the magni tude of the electronic charge. In the present experiments the resistivity was measured by a four-point

¹ E. M. Conwell and V. F. Weisskopf, Phys. Rev. 77, 388 (1950).

² H. Brooks, Phys. Rev. 83, 879 (1951).
³ H. Jones, Phys. Rev. 81, 149 (1951).
⁴ V. A. Johnson and K. Lark-Horovitz, Phys. Rev. 8**2,** 977 (1951).

⁵ F. J. Blatt, Phys. Rev. 105, 1203 (1957).

⁶ F. J. Morin and J. P. Maita, Phys. Rev. 96, 28 (1954).

⁷ P. P. Debye and T. Kohane, Phys. Rev. 94, 724 (1954).

⁸ R. O. Carlson, Phys. Rev. 100, 1075 (1955).

⁹ M.