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The Theory of the Ferromagnetic Anisotropy of Single Crystals

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It is well known that in single crystals of iron and nickel the direction of magnetization is not generally parallel to the direction of the magnetic field, although these crystals belong to the cubic system. When the magnetization in a crystal has a certain value as measured in the direction of the field, there will be also, in general, a component of magnetization measured in the direction at right angles. This paper describes the calculation according to the domain theory, of the normal component of magnetization, using certain assumptions which are almost identical with those used by Heisenberg in his calculation of the magnetostriction of iron crystals. Theoretical curves are shown for a variety of crystallographic directions. Each of these curves shows all of the possible positions and magnitudes of the vector representing the magnetization in iron crystals as the magnetic field parallel to any given direction in the crystal increases in strength from zero to a high value. The theoretical curves are compared with the experimental curves of Honda and Kaya, and show good agreement with them.

INTRODUCTION

RECENTLY Heisenberg[1] has calculated the magneto-striction of a single crystal of iron as dependent upon magnetization, for the three principal directions in the crystal. Restated in my own words, the assumptions used by Heisenberg are as follows:

1. The crystal is composed of a large number of domains, considered for convenience to be equal in size.

2. When the crystal as a whole is in the unmagnetized state, each domain is magnetized to saturation in the direction of a cubic axis, $<100>$, the directions of the magnetizations of the domains being equally distributed among the six possible directions.

3. When magnetization of the crystal as a whole has a value chosen between zero and a certain limit, the directions of magnetizations in the domains are distributed by chance among the six possible $<100>$ directions, and that distribution will occur which is the most probable one, subject to the condition that the vector sum of the magnetizations of the domains shall be equal to the previously specified magnetization of the crystal. The precise meaning of the term probability of a distribution is stated in Eq. (2) below.

4. After magnetization of the crystal has increased so that the directions of magnetizations of the domains have become parallel to that cubic axis (or axes) most nearly aligned with the direction of the magnetic field, as-

[1] W. Heisenberg, Zeits. f. Physik **69**, 287–297 (1931). Similar assumptions were previously stated by W. L. Webster, Proc. Phys. Soc. London **42**, 431–440 (1930), but no quantitative treatment was given nor were calculations made. For a discussion of the domain theory, see E. C. Stover, *Magnetism*, E. P. Dutton and Co., 65–66 (1929), and R. M. Bozorth and J. F. Dillinger, Phys. Rev. **41**, 345 (1932).

sumption (3) no longer applies and they leave the cubic axes and approach the field direction continuously until saturation is attained.

5. Associated with each domain is a measurable "magnetostriction," i.e., a deformation of the domain which increases its length in the direction of its magnetization. The magnetostriction of the crystal is the sum of the separate magnetostrictions of the domains, added according to the method of Akulov.[2]

The magnetostriction curves so calculated for progressive magnetization along the crystallographic directions $<100>$, $<110>$ and $<111>$ have been compared by Heisenberg with the data of Webster[3] and show good agreement with them.

Heisenberg limited himself to the calculation of the *magnetostriction*. On the other hand, by using similar but somewhat different assumptions, and extending his general mathematical procedure, it is possible to predict the *direction of magnetization* in a single crystal subjected to a magnetic field having any chosen direction and magnetized to any fraction of saturation.

It is known experimentally that when the crystal is more than about half saturated the direction of magnetization is different from the direction of the field unless the field lies in one of the three principal crystallographic directions (cube edge, face diagonal, and body diagonal) considered by Heisenberg. As the field increases in strength, remaining always constant in direction, the magnetization changes in direction as well as in magnitude.

We now have a satisfactory theory which predicts correctly in all cases the direction of deviation of magnetization from field, and predicts also within the experimental error the magnitude of the deviation observed by Honda and Kaya, whose experimental data are as yet the most complete.

Specifically, the quantities which are calculated for the first time in this paper are the magnitude and direction of the magnetization in a single crystal corresponding to selected values of the component of magnetization in the field direction. These may be calculated for any direction of the field with respect to the crystal axes.

The assumptions made are assumptions (1) to (4) above, with a slight change in assumption (3): the distribution of the directions of magnetization in the domains is now subject to the condition that the vector sum of these magnetizations shall have a component in the direction of the magnetic field equal to the observed value of the magnetization along that direction.

The simplest way to express the results of the calculations seems to be to plot I_H, the component of magnetization parallel to the field, along one axis; and I_n, the component normal to the field, along an axis at right angles. The line joining the origin to any point on the curve so plotted is then a vector representing the total magnetization of the crystal, and the curve is the locus of the end of the vector as the strength of the field directed along the I_H axis increases from a very small to a very large value. Typical curves are shown in Figs. 4 to 6, where the several directions of the field are shown by the arrows.

[2] N. S. Akulov, Zeits. f. Physik **59,** 254–264 (1930).

[3] W. L. Webster, Proc. Roy. Soc. London **109A,** 570–584 (1925).

It should be understood that the theory gives no information regarding the *strength* of the magnetic field which is associated with a given magnetization of the crystal, but does define completely all of the magnetic states of the crystal which must occur as the field, acting in any direction, increases indefinitely from zero.

CALCULATIONS

Following Heisenberg's procedure, let N denote the number of domains per unit volume of the crystal. We employ a right-handed set of rectangular coordinate axes which coincide with the crystallographic axes. We consider "distributions" of the elementary domains, each distribution being defined by the numbers, N_1, N_3, N_5, of elementary regions per unit volume having their magnetic moments in the directions of the positive x, y and z axes, respectively, and by the numbers N_2, N_4, N_6, of regions having their magnetic moments in the directions of the negative x, y and z axes, respectively. Thus a distribution is represented by a set of positive numbers $(N_1, N_2, \cdots, N_6)$ with $N_1+N_2+\cdots+N_6=N$. The components of the magnetization along the x, y and z axes are then given by

$$\begin{aligned} I_x/I_\infty &= (N_1 - N_2)/N, \\ I_y/I_\infty &= (N_3 - N_4)/N, \\ I_z/I_\infty &= (N_5 - N_6)/N, \end{aligned} \tag{1}$$

respectively, where I_∞ is the saturation value of magnetization. With Heisenberg we write the probability of the distribution $(N_1, N_2, \cdots, N_6)$

$$P(N_1, N_2, \cdots, N_6) = \frac{N!}{(N_1!)(N_2!)\cdots(N_6!)}\left(\frac{1}{6}\right)^N. \tag{2}$$

Imposing the condition that the component of magnetization in the direction defined by direction cosines (λ, μ, ν) has a given value I_H, let us seek the most probable distribution consistent with this condition .We have

$$\lambda(N_1 - N_2) + \mu(N_3 - N_4) + \nu(N_5 - N_6) = NI_H/I_\infty. \tag{3}$$

We also have

$$N_1 + N_2 + \cdots N_6 = N. \tag{4}$$

Introducing Lagrangian multipliers, α' and β, we construct the function

$$\begin{aligned} F = \log P &+ \alpha'[N_1 + N_2 + \cdots N_6 - N] \\ &+ \beta[\lambda(N_1 - N_2) + \mu(N_3 - N_4) + \nu(N_5 - N_6) - NI_H/I_\infty]. \end{aligned} \tag{5}$$

For the most probable distribution we must have

$$\partial F/\partial N_i = 0,\ i = 1, 2, \cdots, 6. \tag{6}$$

Making use of the approximation

$$\log n! = (n + \tfrac{1}{2}) \log n - n + \tfrac{1}{2} \log (2\pi),$$

we obtain from (6) the set of approximate equations

$$\log N_1 = \alpha' + \log (N/6) + \beta\lambda,$$
$$\log N_2 = \alpha' + \log (N/6) - \beta\lambda,$$
$$\log N_3 = \alpha' + \log (N/6) + \beta\mu,$$
$$\log N_4 = \alpha' + \log (N/6) - \beta\mu,$$
$$\log N_5 = \alpha' + \log (N/6) + \beta\nu,$$
$$\log N_6 = \alpha' + \log (N/6) - \beta\nu.$$

Write $\alpha' + \log (N/6) = \alpha$. Then we have

$$\left.\begin{array}{l} N_1 = e^{\alpha+\beta\lambda},\ N_3 = e^{\alpha+\beta\mu},\ N_5 = e^{\alpha+\beta\nu}, \\ N_2 = e^{\alpha-\beta\lambda},\ N_4 = e^{\alpha-\beta\mu},\ N_6 = e^{\alpha-\beta\nu}. \end{array}\right\} \tag{7}$$

On substituting from (7) in (3) and (4), we obtain the following equations for the determination of α and β:

$$\frac{\lambda sh(\lambda\beta) + \mu sh(\mu\beta) + \nu sh(\nu\beta)}{ch(\lambda\beta) + ch(\mu\beta) + ch(\nu\beta)} = \frac{I_H}{I_\infty}, \tag{8}$$

$$2e^{\alpha}[ch(\lambda\beta) + ch(\mu\beta) + ch(\nu\beta)] = N. \tag{9}$$

Eq. (8) gives β in terms of λ, μ, ν, I_H; then (9) gives α in terms of λ, μ, ν, I_H, N. Eqs. (7) then give the most probable distribution (N_1, N_2, $\cdots$, N_6) from which the figures have been plotted.

In Figs. 1 and 2 there are shown the most probable distributions as functions of I_H/I_∞ for two directions (λ, μ, ν). It is to be understood that the preceding theory cannot apply if the value of I_H/I_∞ is greater than that for which one of the N_i's vanishes. In extending the results into the range of these higher values of I_H we make use of assumption (4) of the introduction.

For purposes of comparison with certain experiments it is necessary to discuss cases in which the magnetization I lies always in a given plane. Accordingly, let us impose the conditions that: (1) the component of magnetization in a given direction (λ', μ', ν') be zero, (2) the component in another direction (λ, μ, ν) have a given value I_H; and let us seek the most probable distribution consistent with these conditions.

We have Eqs. (3) and (4) and the additional equation

$$\lambda'(N_1 - N_2) + \mu'(N_3 - N_4) + \nu'(N_5 - N_6) = 0. \tag{10}$$

Proceeding as before, we find the values

$$\begin{array}{l} N_1 = e^{\alpha+\lambda\beta+\lambda'\gamma},\ N_3 = e^{\alpha+\mu\beta+\mu'\gamma},\ N_5 = e^{\alpha+\nu\beta+\nu'\gamma}, \\ N_2 = e^{\alpha-\lambda\beta-\lambda'\gamma},\ N_4 = e^{\alpha-\mu\beta-\mu'\gamma},\ N_6 = e^{\alpha-\nu\beta-\nu'\gamma}, \end{array} \tag{11}$$

where the Lagrangian multipliers α, β, γ, are determined by the equations

$$\lambda' sh(\lambda\beta + \lambda'\gamma) + \mu' sh(\mu\beta + \mu'\gamma) + \nu' sh(\nu\beta + \nu'\gamma) = 0, \tag{12}$$

$$\frac{\lambda sh(\lambda\beta+\lambda'\gamma)+\mu sh(\mu\beta+\mu'\gamma)+\nu sh(\nu\beta+\nu'\gamma)}{ch(\lambda\beta+\lambda'\gamma)+ch(\mu\beta+\mu'\gamma)+ch(\nu\beta+\nu'\gamma)}=\frac{I_H}{I_\infty}, \tag{13}$$

$$2e^{\alpha}[ch(\lambda\beta+\lambda'\gamma)+ch(\mu\beta+\mu'\gamma)+ch(\nu\beta+\nu'\gamma)]=N. \tag{14}$$

Eq. (12) determines γ in terms of β and the direction cosines; then (13) determines β, and so also γ, in terms of the direction cosines and I_H, then (14) gives α in terms of the direction cosines, I_H, and N. Finally the Eqs. (11) give the required most probable distribution.

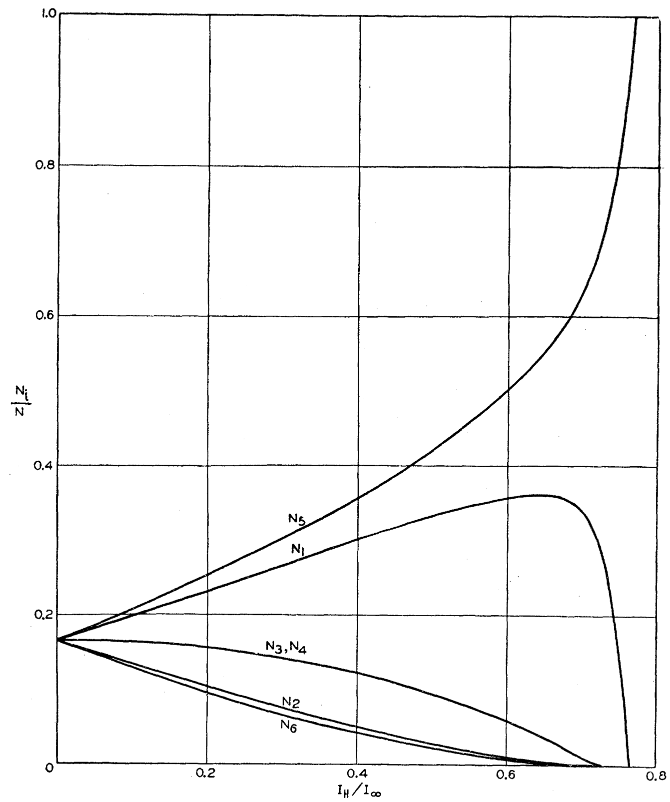

Fig. 1. Curves showing the distribution of directions of magnetizations of the domains among the six <001> directions. For these curves the direction of the field is defined by the direction cosines $\lambda=0.643$, $\mu=0$, $\nu=0.766$, and is therefore inclined at 40° to a <001> direction in a {001} plane.

The curves in Figs. 2 and 3 show the most probable distributions as functions of I_H/I_∞ for one set of values of λ, μ and ν; in the case of Fig. 2 the magnetization is not restricted to a plane, in Fig. 3 it is confined to the $(11\bar{1})$ plane $(\lambda'=\mu'=-\nu'=1/3^{1/2})$.

The results may also be expressed in a different way. From the most probable distributions may be determined I_n, the component of magnetization perpendicular to the direction defined by λ, μ and ν; and therefore knowing

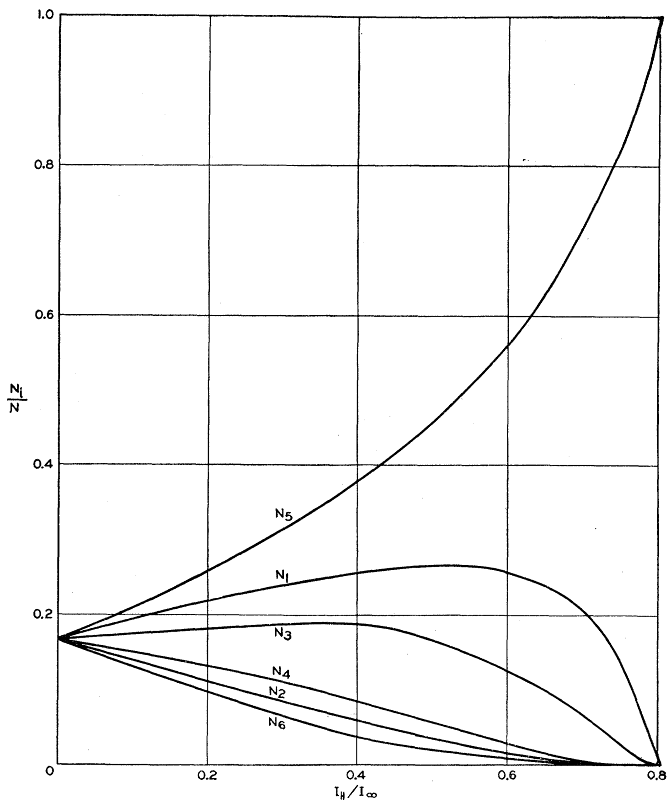

Fig. 2. Distribution curves when the direction of the field has the direction cosines $\lambda=0.525$, $\mu=0.279$, $\nu=0.804$, and therefore lies in the $(11\bar{1})$ plane 10° from the [112] direction. The magnetization is not constrained to lie in the $(11\bar{1})$ plane.

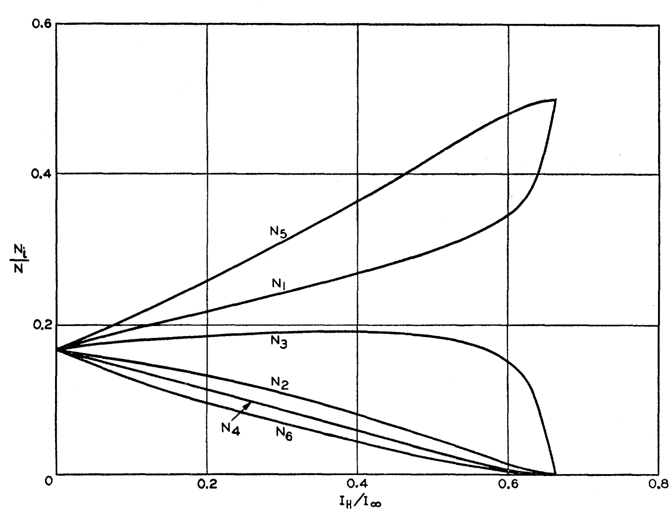

Fig. 3. Distribution curves when the direction of the field is the same as for Fig. 2. The magnetization for this case, however, is confined to the $(11\bar{1})$ plane by the additional condition $N_1-N_2+N_3-N_4-N_5+N_6=0$.

I_H which lies in the latter direction, I may be determined in magnitude and direction. In the polar diagram of Fig. 4, referring to the (001) plane, each curve marked "CALC." is the locus of the end of the vector representing I,

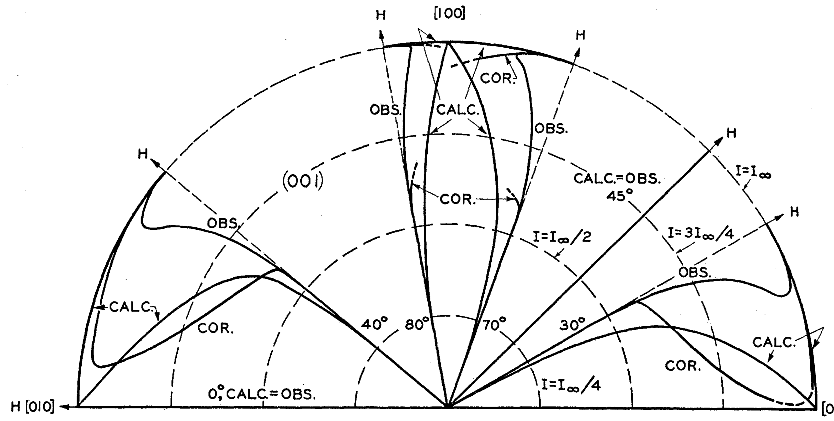

Fig. 4. Polar diagram of magnetization in a {001} plane of iron. Each curve is the path traced from the center of the semi-circle by the end of the vector representing I as I increases in magnitude from zero to I_∞ (the limit of the figure). The direction of the field is that indicated by the arrow, and is the same as the direction of the curve at the origin.

as it passes from the center of the circle to its circumference, while I increases in magnitude from 0 to I_∞. When I_H becomes so large that one of the N_i's

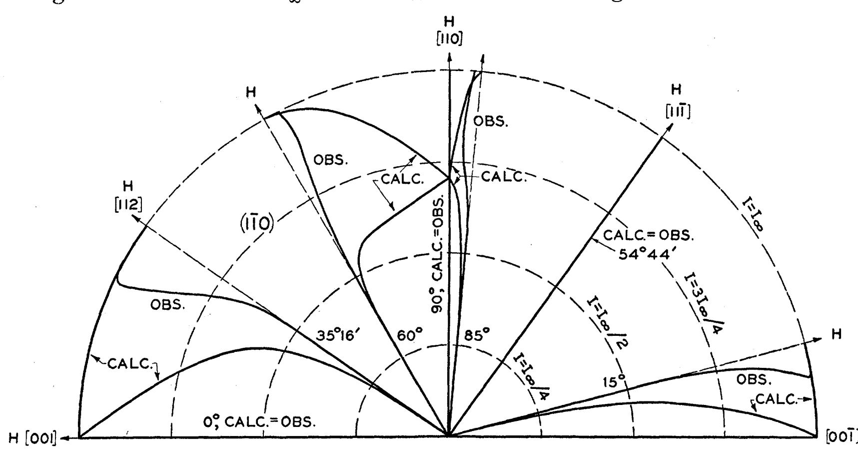

Fig. 5. Polar diagram of magnetization in a {110} plane. The observed curves have not been corrected for the demagnetizing effect of the normal component of magnetization.

vanishes (generally when $I=I_\infty$) it is assumed that I turns in a plane into the direction defined by λ, μ and ν).[4]

The calculated curves shown in Figs. 5 and 6 are similarly determined but

[4] In the special cases where the direction defined by λ, μ and ν makes the same angle with two (or three) of the axes, this last stage begins when $I=I_\infty/2^{1/2}$, (or $I=I_\infty/3^{1/2}$) and it is assumed that each of the two (or three) vectors then directed along the axes turns in a plane into the direction of the field.

are complicated by the fact that I may not equal I_∞ when the redistribution process is complete. In Fig. 6 I does not always lie in the plane of the figure, $(11\bar{1})$. In the latter figure the curve marked "CALC. (1)" is obtained without confining I to the plane, while for curves "CALC. (2)" I is so confined. In Figs. 4 and 5, I is automatically confined to the plane by symmetry.

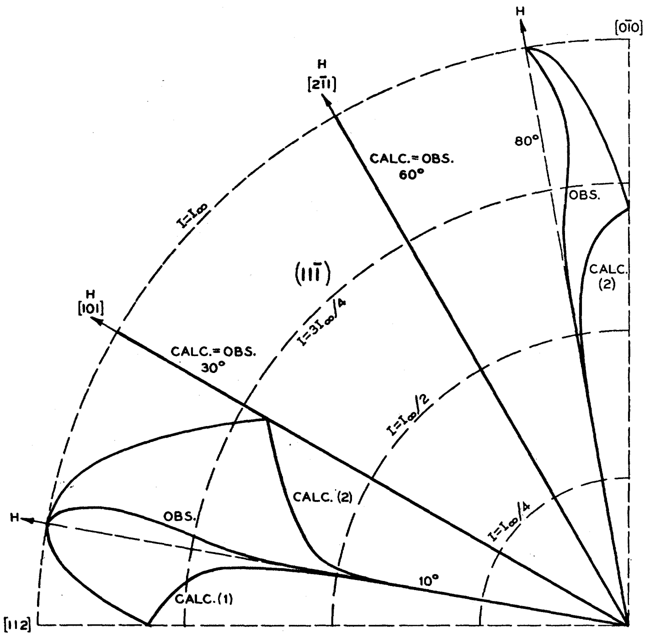

Fig. 6. Polar diagram of magnetization in a $\{111\}$ plane. Curves marked (2) are derived with the magnetization confined to the plane of the figure, corresponding to the experimental data. The observed curves are uncorrected for the demagnetizing effect of the normal component of magnetization.

Comparison with Experiment

The most complete data with which to compare the theoretical results are those of Honda and Kaya,[5] who measured the magnetization parallel and perpendicular to the applied field in an oblate ellipsoid having axes 0.4 mm, 20 mm and 20 mm. From the applied field, they subtract the demagnetizing field acting anti-parallel to the applied field. Considering the resultant field, acting in the same direction as the applied field, to be the effective field, the data are plotted in Figs. 4 to 6 as curves marked "OBS."

These effective fields, however, are not the true magnetic fields acting on the crystal, because no account has yet been taken of the demagnetizing field due to the perpendicular component of the induced magnetization. Proper consideration of this additional field changes considerably the direction of the field which is effective, as shown in Fig. 7. Here the solid arrows are vectors measured from the common point; H' represents the applied field; $H_{H'}$ the field parallel to H' corrected for the demagnetizing field due to the parallel

[5] K. Honda and S. Kaya, Sci. Rep. Tohoku Imp. Univ. (1) **15**, 721 (1926).

component of magnetization $I_{H'}$ shown on a different scale by the dotted line; H_n represents the field due to I_n and equal to I_n multiplied by the demagnetizing factor 0.189, and H represents the (true) field equal to the vector sum of $H_{H'}$ and H_n. This correction has been made to all of the data referring to the (001) plane, and the corresponding curves marked "COR." are shown in Fig. 4. These curves lie much nearer to the calculated curves than the "OBS." curves do, and it is obvious that this correction accounts for most of the original difference between the calculated and experimental results.

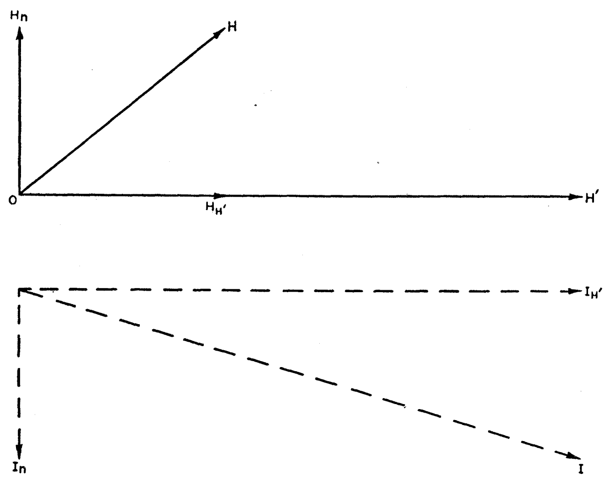

Fig. 7. Vector diagram showing the direction of the (true) field, H, as determined from the applied field, H', and the demagnetizing fields due to the components of magnetization parallel ($I_{H'}$) and perpendicular (I_n) to the applied field.

The corrected curves were derived from the data in the following way. For a given direction of the applied field H', and a certain value of the magnetization $I_{H'}$ parallel to the applied field as taken from the tables of Honda and Kaya, the direction of the field H was determined as indicated in Fig. 7 and the component of I parallel to H, I_H was calculated. This was done for all of the data relating to one direction of the applied field and curves plotted relating both θ_I (the angle between I and a particular $<100>$ axis) and θ_H (the angle between H and the same $<100>$ axis) with I_H. Similar curves were plotted for each of the four directions of the applied field in the (001) plane for which data exist. Selecting a definite value of I_H, these curves were used to obtain values of θ_H and θ_I by interpolation, one pair of values of the latter being obtained for each of the four directions of the applied field for which measurements were made. With the four points so obtained, a curve was plotted relating θ_H and θ_I, with I_H constant. Other curves were similarly plotted with I_H as parameter, and values of θ_I were read from these as a function of I_H for definite values of θ_H and the results plotted as in Fig. 4. This process naturally was subject to inaccuracies due to interpolation, and the final curves are not to be considered as representing the data exactly. Extrapolations of the curves were avoided, and sometimes no values of θ_I could be assigned for certain values of θ_H and I_H, the curves in this case being dotted or omitted entirely.

Because these calculations were rather laborious, they were made only for the (001) plane, but since they show that the curves so corrected lie very much closer to the calculated curves it follows that a similar effect would be noted in the other planes. The correction is always in the right direction.

There is still another limitation in comparing the calculations with experiment. The perpendicular component of magnetization was determined by rotation of the single crystal specimen, so that rotational hysteresis is present. These two factors, hysteresis and the inaccuracy in the determination of the direction of the field on account of the large demagnetizing factor, are sufficient to account for the discrepancies between the corrected and calculated curves. The limitations of the data can easily be noticed when the corrected curve is plotted for $\theta_H = 45°$. Although this curve is not reproduced here it swings to within 20° of the cubic axis when I is about 0.8 of saturation. This deviation of I from the direction of H is known to be in error since the "OBS." curve is a straight line, i.e., there is no perpendicular component when the applied field is in this direction.

The results for the $(11\bar{1})$ plane are particularly interesting, for if H lies in this plane I will generally not do so. When H is inclined 10° to the [211] direction, curve marked "CALC. (1)" in Fig. 6 indicates that the theory predicts an effect in the direction opposite to that observed. In the extremely oblate ellipsoid used in the experiments, however, the magnetization is constrained to lie almost completely in the plane. When this condition is added to the others in the mathematical expression of the theory as described in the preceding section (Eqs. (10) et seq.), the direction of the perpendicular component is the same as that observed, as shown in curve "CALC. (2)."

The agreement between theory and experiment seems to be within the experimental error.

Discussion

In making the calculations and plotting the results in the figures, nothing has been said explicitly about the magnitude of the magnetic field H which in the actual experiment induces the magnetization. The energy associated with each of the six directions of easy magnetization is supposed to be the same irrespective of the magnitude or direction of the field. The field is influential only in producing a magnetization having a component of given magnitude parallel to the field, the component at right angles being determined by probability considerations. There is little question but that this supposition is justified when the magnetization is small, perhaps even when it is as large as one-half of its saturation value, for then the corresponding field-strength is known to be small compared to the internal or molecular fields and cannot change the distribution function appreciably. On the other hand, when I becomes equal to I_∞ the probability considerations no longer apply and the vector representing I_∞ is assumed to turn slowly into the direction of the field, remaining always in the same plane.[6]

[6] R. Gans, following a proposal of Heisenberg's, has recently indicated how to calculate the position of this vector as dependent upon the field strength. Phys. Zeits. **33**, 15 (1932).

The transition between these two situations is undoubtedly not perfectly sharp, and it may be expected that a more complete calculation, taking account of the magnitude of the field, would show the curves to be rounded at the point of contact with a $<100>$ axis instead of sharp as shown in the figures.

Akulov[2] has made an extended theoretical study of the ferromagnetic properties of crystals, and has based many of his conclusions on the assumption that the magnetization in a domain may have any direction with respect to the crystal axes—that the domain is magnetically isotropic—as long as the magnetization is less than half of the saturation value. This assumption was made because experiments have shown the magnetization perpendicular to the field to be small or zero when the total magnetization of the crystal is less than half of saturation. Our theory accounts for this experimental fact but is based on the contrary assumption that the domains are saturated in a $<100>$ direction even for the smallest values of the crystal magnetization. Thus it is unnecessary to accept Akulov's rather artificial picture of isotropic domains suddenly becoming anisotropic when the magnetization of the crystal exceeds a critical value. The curves of Figs. 4 to 6 show how slight is the difference between the directions of H and I when $I<I_\infty/2$. The difference between the calculated and observed curves in this region may well be due to the inaccuracy of the data, for it is in this region of small field strengths that the demagnetizing action of the perpendicular component, discussed at length above, is a maximum. Rotational hysteresis also would tend to make the observed perpendicular component too small.

Powell[7] has proposed a theory of the magnetic anisotropy of crystals which expresses the direction of the magnetization as a function of the magnitude and direction of the field. When the field is applied in a $\{111\}$ plane of iron or nickel, however, and the magnetization is constrained also to lie in that plane, his theory requires that I should be parallel to H. The data show that the degree of anisotropy is smaller than in the other planes, but still it appears quite definite, especially for iron. On the other hand, my theory indicates that in this plane and under this condition there should be a deviation of I from H in the observed direction and approximately of the observed amount. This casts considerable doubt on the validity of Powell's theory. Mahajani's[8] theory is also open to the same objection. It may be mentioned that in comparing his theory with experiment, Powell considered the field H to coincide in direction with the applied field, whereas in general their directions are different as remarked above.

The theory may obviously be applied to nickel, in which the directions of easy magnetization are $<111>$ instead of $<100>$ as in iron.

I take pleasure in expressing my indebtedness to L. A. MacColl for the mathematical work of the second section.

[7] F. C. Powell, Proc. Roy. Soc. London **130A**, 167–181 (1930).
[8] G. S. Mahajani, Phil. Trans. Roy. Soc. London **228**, 63–114 (1929).