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MONOTONIC MAGNETOSTRICTION FOR NONFERROMAGNETIC MATERIALS

by Lawrence Flax

Lewis Research Center
Cleveland, Ohio

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SUMMARY

The constant magnetostriction coefficient for nonferromagnetic materials is derived in terms of changes in the Fermi surface. The theory is applied to Fermi surfaces of spherical and elliptical geometries. The magnetostriction coefficient along the trigonal axis of bismuth is calculated and compared with experimental results.

INTRODUCTION

The magnetostriction of nonferromagnetic materials was first observed by Kapitza (ref. 1) for large transient fields. Subsequently, Shoenberg (ref. 2), Wolf and Goetz (ref. 3), Anderholm (ref. 4), and Aron (unpublished NASA data) investigated this phenomenon. These investigators observed that magnetostriction was a function of crystal direction relative to the field and was dependent on the first power of the magnetic field. The phenomenon was assumed to arise from the change of magnetization, which provides the energy for elastic deformation.

The magnetostriction coefficient of a sample in a homogeneous magnetic field is defined as the fractional change in length per unit magnetic field. The magnetostriction is called longitudinal or transverse depending on whether the change in length is measured in the direction of the magnetic field or perpendicular to it.

In classical physics, a system of free electrons confined to a fixed volume has zero diamagnetic moment. In quantum mechanics, the quantization of angular momentum in a magnetic field results in a nonzero magnetic moment. The magnetization is composed of two components, one of which is constant and the other is oscillatory with respect to changes in magnetic field. This report is concerned only with the constant component of the diamagnetic moment.

The constant component of magnetization is formed chiefly from the bunching of energy levels. The application of a magnetic field does not, however, change the average density of the levels. The magnetostriction coefficient, which depends on the magnetization, is derived in terms of the effect of an elastic deformation on the extremal area of the Fermi surface. This deformation is caused by a change in both the equilibrium electron density and the energy of the electrons.

In general, an electron in a metal is governed by a complicated dispersion law. The frequently used quadratic dispersion law for conduction electrons is valid only when the Fermi surface is the lower part of the Brillouin zone. The theory presented in this report can be applied to an arbitrary dispersion law.

SYMBOLS

C	longitudinal magnetostriction
c	speed of light
E	electron energy
E_o	electron energy in undeformed state
E'	electron energy in deformed state
e	electron charge
$f\frac{(E-\rho)}{kT}$	Fermi distribution function
$g(\rho)$	density of states
H	magnetic field
$\hbar$	Plank's constant divided by 2π
K	compressibility (isotropic), $S_{ijk\ell}\delta_{ij}$
K_{ij}	deformation parameter
k	Boltzmann constant
$\vec{k}$	wave number
k_n	normal displacement of Fermi surface in $\vec{k}$ space
k_o	radius of spherical Fermi surface
ℓ	deformed length
ℓ_o	undeformed length
M	magnetization per unit volume
M_T	temperature component of magnetization
m_{ij}	effective mass tensor element

m_o	mass of free electron
n	number of electrons per unit volume
n_o	number of electrons per unit volume in undeformed state
P	pressure
p	electron momentum
p_o	extremal momentum
p_z	electron momentum in z-direction
R	summation index
S	cross-sectional Fermi surface area
$S_{ijk\ell}$	compliance tension element
S_m	extremal cross-sectional area of Fermi surface
T	temperature
V	volume of sample
V_F	Fermi velocity
α_{ij}	m_o/m_{ij}
β_{ij}	hole effective mass
γ	phase
γ_{ij}	directional cosines
Δ	dilation
δ	see equation (8)
δ_{ij}	Kronecker delta function
ρ	chemical potential
ρ_o	chemical potential in undeformed state
$\sigma_{k\ell}$	stress tensor element
ω_{ij}	strain tensor element

THEORETICAL ANALYSIS

The longitudinal magnetostriction coefficient developed from thermodynamics (ref. 5) is given by

$$C = \frac{1}{\ell_o}\left(\frac{\partial \ell}{\partial H}\right)_{T,\sigma} = +MK - \left(\frac{\partial M}{\partial \sigma}\right)_{H,T} \tag{1}$$

The first term of equation (1) gives an extremely small contribution (about 10^{-22}) per gauss. Therefore, the magnetostriction coefficient is very closely given by

$$C = -\left(\frac{\partial M}{\partial \sigma}\right)_{H,T} \tag{2}$$

The constant diamagnetic component of the magnetization of an electron gas as given by Lifshitz and Kosevich (ref. 6) is

$$M = \frac{2}{\pi^3}\frac{e^2}{\hbar c^2} H \left(\sum_{R=1}^{R=\infty} \frac{\sin 2\pi R\gamma - \cos 2\pi R\gamma}{R^2}\right) \int_0^\infty \frac{f\left(\frac{E - \rho}{kT}\right)}{\frac{\partial S(E, p)}{\partial p_o}} dE \tag{3}$$

where

$$f(x) \equiv \left(1 + e^x\right)^{-1}$$

and $\partial S/\partial p_o$ is a derivative of S with respect to p evaluated at the extremal momentum. For $kT << \rho$, equation (3) becomes

$$M = \frac{2}{\pi^3}\frac{e^2}{\hbar c^2} H \sum_{R=1}^{R=\infty} \frac{\sin 2\pi R\gamma - \cos 2\pi R\gamma}{R^2}\left[\int_0^\rho \frac{dE}{\frac{\partial S}{\partial p_o}} + \frac{\pi^2}{6}(kT)^2 \frac{d}{dE}\left(\frac{\partial S}{\partial p}\right)^{-1}\right] \tag{4a}$$

For $T \approx 0$, the second term in brackets contributes very little, and therefore,

$$M = \frac{2}{\pi^3}\frac{e^2}{\hbar c^2} H \sum_{R=1}^{R=\infty} \frac{\sin 2\pi R\gamma - \cos 2\pi R\gamma}{R^2}\int_0^\rho \frac{dE}{\frac{\partial S}{\partial p_o}(E, p_o)} \tag{4b}$$

If a function φ is considered, where

$$\varphi \equiv \int_{t_2(\alpha)}^{t_1(\alpha)} F(X, \alpha) dX$$

then,

$$\frac{\partial \varphi}{\partial \alpha} = \int_{t_2(\alpha)}^{t_1(\alpha)} \frac{\partial F(X, \alpha)}{\partial \alpha} dx - F(t_2, \alpha) \frac{dt_2}{d\alpha} + F(t_1, \alpha) \frac{dt_1}{d\alpha}$$

and equation (4b) becomes,

$$C = - \left(\frac{\partial M}{\partial \sigma}\right)_{H, T} = - \frac{2}{\pi^3 \hbar c^2} \sum_{R=1}^{R=\infty} \frac{\sin 2\pi R\gamma - \cos 2\pi R\gamma}{R^2} \frac{\partial \rho}{\partial \sigma} \frac{1}{\frac{\partial S(\rho, p_o)}{\partial p_o}} \tag{5}$$

To determine the component $\partial\rho/\partial\sigma$, the following reasoning is applied. The magnetic field disturbs the lattice, moving the atoms away from the position of zero field equilibrium and thereby deforming the Fermi surface and changing the value of ρ. It is assumed that the influence of an elastic deformation of the latter can be taken into account in the form of a small addition to the electron energy proportional to the deformation tensor. This assumption implies that the energy of the electrons after deformation is

$$E(\vec{k}) = E_o(\vec{k}) + E'(\vec{k}) \tag{6}$$

where $E(\vec{K})$, $E_o(\vec{K})$ are the electron energies in the deformed and undeformed metal, respectively, and $E'(\vec{k})$ is the change in the energy of the electrons due to a deformation.

Assuming the number of electrons is constant and using equation (6), Ziman (ref. 7) showed that the change in the chemical potential is

$$\Delta\rho = - \left[\frac{n_o(\rho_o)}{g(\rho_o)} \delta_{ij} - E'\right] \omega_{ij} \tag{7}$$

The changes involved in the energy surfaces may be described by a deformation tensor $K_{ij}(\vec{k})$ introduced by Pippard (ref. 8). This tensor is defined by

$$\delta k_n = \omega_{ij} K_{ij}(\vec{k}) \tag{8}$$

where ω_{ij} is the strain tensor element and δk_n is the normal displacement of the Fermi surface. The right side of equation (8) represents the sum of the nine terms that results from summing the dummy indices i and j over the range of values 1, 2, and 3.

Under a deformation, the energy of an electron is changed by the amount

$$E' = \left[\nabla_k(E)\right]\delta k_n \tag{9}$$

With equation (8), E' can be written as

$$E' = \hbar V_F(\vec{k}) K_{ij}(\vec{k})\omega_{ij} \tag{10}$$

Substitution of equation (10) into equation (7) leads to

$$\delta\rho = -\left[\frac{n_o(\rho_o)}{g(\rho_o)}\,\delta_{ij} - \hbar V_F(\vec{k})\,K_{ij}(\vec{k})\right]\omega_{ij} \tag{11}$$

If the generalized form of Hook's law $\omega_{ij} = S_{ijk\ell}\sigma_{k\ell}$ is used, where $S_{ijk\ell}$ is the elastic compliance tensor, the change in chemical potential with stress can be written as

$$\begin{aligned}\frac{\partial\rho}{\partial\sigma_{k\ell}} &= -\left[\frac{n_o(\rho_o)}{g(\rho_o)}\,\frac{1}{V}\,\frac{\partial V}{\partial p} - \hbar V_F(\vec{k}) K_{ij}(\vec{k}) S_{ijk\ell}\right] \\ &= \left[\frac{n_o(\rho_o)}{g(\rho_o)}\,K + \hbar V_F(\vec{k}) K_{ij}(\vec{k}) S_{ijk\ell}\right]\end{aligned} \tag{12}$$

Hence, from equation (5),

$$C = -\frac{2V}{\pi^3}\,\frac{e^2 H}{\hbar c^2}\sum_{R=1}^{R=\infty}\frac{\sin 2\pi R\gamma - \cos 2\pi R\gamma}{R^2}\;\frac{1}{\dfrac{\partial S(E, p_o)}{\partial p_o}}\left[\frac{n_o(\rho_o)K}{g(\rho_o)} + \hbar V_F(\vec{k})\,K_{ij}(\vec{k})\,S_{ijk\ell}\right] \tag{13}$$

For temperatures above $T = 0$, the second term in equation (4a) must be included, and this gives the contribution

$$M_T = -\frac{1}{3}\,\frac{e^2VH(KT)^2}{\hbar c^2}\sum_{R=1}^{R=\infty}\frac{\sin 2\pi R\gamma - \cos 2\pi R\gamma}{R^2}\,\frac{\partial^2 S(E, p_o)}{\partial p_o\,\partial E}\left[\frac{\partial S(E, p_o)}{\partial p_o}\right]^{-2} \tag{14}$$

Hence, the temperature component of magnetostriction coefficient can be written as

$$C = \frac{1}{3}\,\frac{e^2VH(KT)^2}{\hbar c^2}\sum_{R=1}^{R=\infty}\frac{\sin 2\pi R\gamma - \cos 2\pi R\gamma}{R^2}\,\frac{\partial}{\partial\sigma}\left\{\frac{\partial^2 S(E, p_o)}{\partial p_o\,\partial E}\left[\frac{\partial S(E, p_o)}{\partial p_o}\right]^{-2}\right\} \tag{15}$$

APPLICATIONS

The longitudinal magnetostriction coefficient is computed for two cases. As an example of a spherical Fermi surface, sodium is used, and for other alkali metals, $\gamma = 1/2$; hence,

$$\sum_{R=1}^{R=\infty}\frac{\sin 2\pi R\gamma - \cos 2\pi R\gamma}{R^2} = \frac{\pi^2}{12} \tag{16}$$

$$\frac{n_o(\rho_o)}{g(\rho_o)} = \frac{2}{3}\,\rho_o = \frac{\int_S \frac{dS\,dE}{V_F}}{\int_S \frac{dS}{V_F}} \tag{17}$$

$$S = 2\pi m_o\left(E - \frac{P_z^2}{2m_o}\right) \tag{18}$$

$$\frac{\partial S}{\partial p} = -2\pi\left(2m_o\right)^{1/2} \tag{19}$$

For a spherical Fermi surface,

$$K_{ij} = \frac{1}{3} \delta_{ij} k_o \tag{20}$$

where k_o is the radius of the Fermi surface.

Inserting the previous values into equation (13) yields

$$C = \frac{1}{6\pi} + \frac{1}{9\pi^2} \frac{e^2 HK\rho_o^{1/2}}{\hbar(2m_o)^{1/2}} \tag{21}$$

where

$$k = 156 \text{ cm}^2/\text{dyne}$$

$$\rho_o = 3.2 \text{ eV}$$

therefore, $C/H = 1.85 \times 10^{-18}$, which is too small to be observed experimentally.

ELLIPSOIDAL FERMI SURFACE FOR BISMUTH

Before calculating the coefficient of magnetostriction, it is advantageous to explain some of the salient features of bismuth. Bismuth has five electrons per atom and is classified as a semimetal. This metal has a small number of free electrons due to overlap outside the Brillouin zone. It is believed that the Fermi surface of bismuth consists of highly anisotropic ellipsoids.

No detailed calculation of the energy bands of bismuth has been made. Thus, it is impossible to determine $K_{ij}(\vec{k})$ and effective mass analytically, but it may be possible to evaluate them by experimental techniques. Fortunately, a large amount of experimental information has accumulated on the band structure of bismuth. Measurements of the de Haas - Van Alphen cyclotron resonance and ultrasonic attenuation can be interpreted in terms of a simple model of ellipsoidal energy surfaces. An interpretation of the de Haas - Van Alphen experiments for electrons has shown that the axis of an ellipsoid is not along but is tipped out of the principle symmetry axis of the crystal. Other models propose more than three electron ellipsoids; usually they assume six ellipsoids. Most of these models have one factor in common, which is that some of the ellipsoids are associated with holes and some with electrons. The question of the correct model for bismuth has not yet been resolved.

Recent investigations by Aron (unpublished data), and Brandt and Venttsel (ref. 9) have indicated that some of the physical properties for bismuth, such as the amplitudes on the trigonal direction of oscillatory magnetostriction and very low temperature de Haas - Van Alphen effects, come from the hole ellipsoid.

By measuring electrical resistivity and the Hall coefficient, Jain and Jagge (ref. 10) determined that $\hbar V(\vec{k})K_{ij}(\vec{k})$ along the trigonal axis is about 2.5 electronvolts.

In order to calculate the magnetostriction coefficient, two models are employed. For the first model the following assumptions are made:

(1) The electron ellipsoids contribute negligibly to magnetostriction.

(2) The term $\hbar V(\vec{k})K_{ij}(\vec{k})$ is due only to the hole contribution.

(3) The hole contribution consists of two identical hole ellipsoids.

When the constant energy surfaces are no longer spherical, a scalar effective mass does not apply. Since equation (19) can no longer be used, equation (13) must be referred to. The hole ellipsoid is described by the dispersion law

$$2m_o\rho_h = \beta_{11}P_x^2 + \beta_{22}P_y^2 + \beta_{33}P_z^2 \tag{22}$$

The extremal area $S_m(\rho_h)$ of cross section of the ellipsoid can be evaluated by analytic geometry from equation (22) to be

$$S_m(\rho) = \frac{2m_o\rho_h}{\lambda_h^{1/2}} \tag{23}$$

where

$$\lambda_h = \gamma_{11}^2(\beta_{22}\beta_{33}) + \gamma_{22}^2(\beta_{11}\beta_{33}) + \gamma_{33}^2(\beta_{11}\beta_{22})$$

and γ_{ii} are the directional cosines that depend on the orientation of the magnetic field, and the subscripts on λ refer to the holes. In the following, the theory of the case where the field is parallel to the trigonal axis is applied.

The area of the curve of constant energy is obtained by using the Bohr - Sommerfeld quantization condition and can be shown to be

$$S(\rho_h, P_z) = \oint\oint dP_x\, dP_y = \left(n + \frac{1}{2}\right)\frac{2\pi\hbar eH}{c} = S_m(\rho_h)\left[1 - \frac{\pi P_z^2\beta_{11}\beta_{22}\beta_{33}}{S_m(\rho_h)\lambda^{3/2}}\right] \tag{24}$$

Hence, the following can be obtained:

$$\frac{\partial S(\rho_h, P_o)}{\partial P_o} = \left.\frac{\partial S(\rho_h, P_z)}{\partial P_z}\right|_{P_o} = \frac{-2\pi P_z \beta_{33}}{\sqrt{\beta_{11}\beta_{22}}} = \frac{-2\pi \sqrt{2m_o}\ \rho_h \sqrt{\beta_{33}}}{\sqrt{\beta_{11}\beta_{22}}} \tag{25}$$

From quantum mechanical considerations γ is restricted to the range $0 < \gamma < 1$. For the case of a quadratic dispersion law $\gamma = 1/2$, and for other Fermi surfaces γ differs from 1/2.

Using the experimental data obtained by Jaggi and Jain (ref. 10) for the term $\hbar V(\vec{k})K_{ij}(\vec{k})$ and substituting equation (24) into equation (13) as well as summing over the two ellipsoids yield

$$\frac{C}{H} = \frac{2e^2\sqrt{\beta_{11}\beta_{22}}}{12\pi^2\hbar C^2\sqrt{2m_o\rho_h}\sqrt{\beta_{33}}}\left[\frac{2}{3}\rho_o K + K_{ij}(\vec{k})\hbar V_F(\vec{k})S_{ijk\ell}\right] = 1.76\times10^{-16} \tag{26}$$

For the second calculation, the nontilted eight ellipsoid model proposed by Abeles and Meiboom (ref. 11) will be used. This model proposes two hole ellipsoids and six electron ellipsoids. For this case, the assumption employed will be that the holes and electrons contribute equally to the term $\hbar V(\vec{k})K_{ij}(\vec{k})$. Using equations (21) to (24) and substituting ρ_e and α_{ij} produces the electron's Fermi energy and the electron's effective mass for ρ_h and β_{ij}, respectively. Summing over the eight electron ellipsoids yields the following:

$$\frac{C}{H} = \frac{6e^2\sqrt{\alpha_{11}\alpha_{22}}}{12\pi^2\hbar C^2\sqrt{2m_o\rho_e}\ \sqrt{\alpha_{33}}}\left[\frac{2}{3}\rho_o K + \frac{K_{ij}(\vec{k})\hbar V_F(\vec{k})S_{ijk\ell}}{2}\right] \tag{27}$$

To obtain the two hole ellipsoid contribution equation (25) is employed. The magnetostriction coefficient for this model is, therefore,

$$\frac{C}{H} = \frac{2e^2\sqrt{\beta_{11}\beta_{22}}}{12\pi^2\hbar C^2\sqrt{2m_o\rho_h}\ \sqrt{\beta_{33}}}\left[\frac{2}{3}\rho_h K + \frac{K_{ij}(\vec{k})\hbar V_F(\vec{k})S_{ijk\ell}}{2}\right]$$

$$+ \frac{6e^2\sqrt{\alpha_{11}\alpha_{22}}}{12\pi^2\hbar C^2\sqrt{2m_o\rho_e}\sqrt{\alpha_{33}}}\left[\frac{2}{3}\rho_e K + \frac{K_{ij}(\vec{k})\hbar V_F(\vec{k})S_{ijk\ell}}{2}\right]$$

$$= 1.84\times10^{-16} \tag{28}$$

A factor of 2 appearing in the term $[\hbar V_F(\vec{k})K_{ij}(\vec{k})S_{ijk\ell}]/2$ is due to the assumption that the electrons and holes contribute equally.

From cyclotron resonance, de Haas - Van Alphen, and ultrasonic attenuation data (ref. 12), the following values are obtained:

$$\alpha_{11} = 2.02$$

$$\alpha_{22} = 1.67$$

$$\alpha_{33} = 83.3$$

$$\rho_e = 2.9\times10^{-14} \text{ erg}$$

$$\rho_h = 2.6\times10^{-14} \text{ erg}$$

$$S_{ijk\ell} = 4\times10^{-12} \text{ cm}^2/\text{dyne}$$

$$K = 3.2\times10^{-12} \text{ cm}^2/\text{dyne}$$

$$\beta_{11} = 2.0$$

$$\beta_{22} = 2.0$$

$$\beta_{33} = 1.4$$

$$\left(\frac{C}{H}\right)_{trig} = 1.76\times10^{-16}$$

$$\frac{C}{H}\text{ (electron + holes)} = 1.86\times10^{-16}$$

The experimental values of C/H are reported in table I.

TABLE I. - RATIO OF LONGITUDINAL

MAGNETOSTRICTION TO MAGNETIC

FIELD IN TRIGONAL DIRECTION

Source	Trigonal values of C/H
Wolf and Goetz (ref. 3)	5.7×10^{-16}
Kapitza (ref. 4)	6.5
Anderholm (ref. 4)	8.3
Aron (unpublished NASA data)	7.2

CONCLUSIONS

The theory presented for the magnetostriction coefficient cannot be accurately tested for bismuth. In order for the theory to be adequately employed, a band calculation for this metal must be made. An alternate procedure would be to obtain sufficient experimental data on the deformation parameter for bismuth.

If this theory is correct, the value of the magnetostriction coefficient C depends basically on two quantities: the change of Fermi surface area with momentum, and the deformation parameter. If the deformation parameter $K_{ij}(\vec{k})$ can be evaluated from theoretical calculations and C can be determined from experimental measurements, the phase factor γ may be determined for complicated surfaces.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, May 12, 1966,
129-02-05-09-22.

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