Stability of One-Dimensional Ferromagnetic Microstructures*

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The equilibrium equations for the distribution of magnetization directions in a *homogeneous* ferromagnetic body possess one-dimensional solutions with some resemblance to a domain structure. It is shown here that under strictly one-dimensional conditions, which are possible only in an infinite plane plate, all the solutions in which the magnetization is not uniform are unstable, and that the Bloch wall acquires its stability from three-dimensional considerations implicit in the initial formulation of the problem.

1. INTRODUCTION

IN a ferromagnet at a specified temperature T and in a specified applied field $\mathbf{H}_0$, the vector magnetization $\mathbf{M}$ has a fixed magnitude M_s but a direction that may vary with position. The condition for stable equilibrium is that the thermodynamic potential G corresponding to choice of T and $\mathbf{H}_0$ as independent variables (the Gibbs free energy) shall be a minimum with respect to the direction cosines α_1, α_2, and $\alpha_3=\pm(1-\alpha_1^2-\alpha_2^2)^{\frac{1}{2}}$ of $\mathbf{M}$. Mere equilibrium, without regard to stability, requires only that G be stationary, i.e., that its first variation vanish; this requirement leads to nonlinear partial differential equations and boundary conditions.[1] One-dimensional analytic solutions exist in certain cases and resemble observed domain structures.[2,3] It is therefore important to find whether the equilibrium in these states is stable, i.e., whether the second variation of G is positive (or at least non-negative) for arbitrary variations of α_1 and α_2.

We shall investigate solutions obtained under the constraint that there is variation with only one Cartesian coordinate, z. Such a strictly one-dimensional situation can exist only in an infinite plate bounded by planes $z=\text{const}$; we shall suppose that the plate occupies the region $z_1\leq z\leq z_2$. In a homogeneous plate in a uniform applied field, the equilibrium equations have uniform solutions $\alpha_i=\text{const}=\alpha_{i0}$. They also have, at least in certain cases, non-uniform solutions $\alpha_i=\alpha_i(z)$; this will be shown in Sec. 2. We shall show that all the non-uniform solutions are unstable. We shall then discuss the implications of this theorem with respect to the Bloch wall and to the effect of imperfections.

2. EQUILIBRIUM CONDITIONS

For unit area normal to Oz,

$$G=\int_{z_1}^{z_2} L(\alpha_1',\alpha_2',\alpha_1,\alpha_2)dz, \tag{1}$$

where

$$L(\alpha_1',\alpha_2',\alpha_1,\alpha_2)=\tfrac{1}{2}C[\alpha_1'^2+\alpha_2'^2+\alpha_3'^2]+f_1(\alpha_1,\alpha_2)-M_s(H_{0x}\alpha_1+H_{0y}\alpha_2+H_{0z}\alpha_3)-\tfrac{1}{2}\mathbf{M}\cdot\mathbf{H}'. \tag{2}$$

Here $\alpha_i'=d\alpha_i/dz$; C is an exchange constant, f_1 is the crystalline-anisotropy energy, and $\mathbf{H}'$ is the field intensity of the poles due to $\mathbf{M}$. The term $-\frac{1}{2}\mathbf{M}\cdot\mathbf{H}'$ represents magnetostatic self-energy. It is not an energy density; its integral over any volume V gives, within the limitations of the Lorentz local-field formula,[4] the mutual energy of pairs of dipoles inside V, plus half the mutual energy of pairs of which one member is inside V and the other outside. In one-dimensional variational procedures, this term yields the correct torques; but its physical meaning must not be forgotten.

The pole distributions are uniform layers normal to Oz. Therefore by elementary magnetostatics

$$H'_x=H'_y=0, \quad H'_z=-4\pi M_z, \tag{3}$$

and

$$-\tfrac{1}{2}\mathbf{M}\cdot\mathbf{H}'=2\pi M_z^2=2\pi M_s^2\alpha_3^2; \tag{4}$$

the magnetostatic self-energy is equivalent to an anisotropy energy of density $2\pi M_s^2\alpha_3^2$, which favors magnetization normal to Oz.

In a homogeneous crystal in a uniform applied field, G is a minimum for uniform magnetization along a direction that minimizes the effective anisotropy-energy density

$$f(\alpha_1,\alpha_2)=f_1(\alpha_1,\alpha_2)-M_s(H_{0x}\alpha_1+H_{0y}\alpha_2+H_{0z}\alpha_3)+2\pi M_s^2\alpha_3; \tag{5}$$

$f(\alpha_1,\alpha_2)$ includes the effects of external and internal fields. Because of the positive definite character of the

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exchange term in L, non-uniform equilibrium states can be at most metastable. Our problem is to find whether they are metastable or unstable.

In terms of α_1 and α_2,

$$L=\tfrac{1}{2}[m_{11}\alpha_1'^2+2m_{12}\alpha_1'\alpha_2'+m_{22}\alpha_2'^2]+f, \quad (6)$$

where the m_{ij}'s are functions of α_1 and α_2. The first variation of G is

$$\delta G=\int_{z_1}^{z_2}\sum_{i=1}^{2}\left(\frac{\partial L}{\partial\alpha_i'}\delta\alpha_i'+\frac{\partial L}{\partial\alpha_i}\delta\alpha_i\right)dz$$

$$=\left(\sum_{i=1}^{2}\frac{\partial L}{\partial\alpha_i'}\delta\alpha_i\right)\Bigg|_{z_1}^{z_2}+\int_{z_1}^{z_2}\sum_{i=1}^{2}\left(-\frac{d}{dz}\frac{\partial L}{\partial\alpha_i'}+\frac{\partial L}{\partial\alpha_i}\right)\delta\alpha_i dz. \quad (7)$$

The equilibrium conditions are found by equating to zero the coefficients of $\delta\alpha_1$ and $\delta\alpha_2$ in the integral and in each boundary term. This gives the differential equations

$$\frac{d}{dz}\frac{\partial L}{\partial\alpha_i'}-\frac{\partial L}{\partial\alpha_i}=0, \quad (i=1, 2) \quad (8)$$

and the boundary conditions

$$\partial L/\partial\alpha_i'=0 \text{ at } z=z_1 \text{ or } z_2, \quad (i=1, 2). \quad (9)$$

From Eq. (9), because of the positive-definiteness of (m_{ij}),

$$\alpha_i'=0 \text{ at } z=z_1 \text{ or } z_2, \quad (i=1, 2). \quad (10)$$

Equations (8) are identical with Lagrange's equations of motion, and G with Hamilton's integral, for a particle of mass C and Cartesian coordinates α_1, α_2, α_3, constrained to move on the unit sphere under the influence of forces derivable from a potential energy $-f(\alpha_1,\alpha_2)$ (note the minus sign); in this dynamic analog, z is time. In the derivation of Lagrange's equations by variation of Hamilton's integral, the positions at times z_1 and z_2 are held fixed, whereas in our magnetic problem $\alpha_i(z_1)$ and $\alpha_i(z_2)$ are free to vary; consequently our variational procedure yields boundary conditions as well as differential equations. Solutions of the magnetic problem correspond, in the dynamic analog, to motions in which the particle is released from rest at time z_1 from such a position that it just comes to rest at time z_2. In simple cases, such as the case $f=K\alpha_3$ (motion of a spherical pendulum in the earth's gravitational field), the possible motions include periodic motions between points of instantaneous rest, with periods dependent on the amplitude; thus nonuniform solutions of the magnetic problem exist at least for some forms of f and for some values of z_2-z_1. An inhomogeneous specimen, in which the anisotropy constants vary with z, corresponds to motion in a force field with time-dependent potential. We consider only the homogeneous specimen.

For a uniform solution, α_i'' as well as α_i' vanishes at each boundary; then from the differential equations, $\partial f/\partial\alpha_1=\partial f/\partial\alpha_2=0$ at the boundaries. Conversely, a solution with $\alpha_1''=\alpha_2''=0$ or with $\partial f/\partial\alpha_1=\partial f/\partial\alpha_2$ at a boundary must be a uniform solution. This is obvious from the dynamic analog: a particle with zero initial acceleration as well as zero initial velocity is at rest at an extremum of potential energy and will remain so. In examining the non-uniform solutions, therefore, we may assume that α_1'' and α_2'', or $\partial f/\partial\alpha_1$ and $\partial f/\partial\alpha_2$, do not both vanish at a boundary.

3. INSTABILITY OF THE NONUNIFORM SOLUTIONS

Under the conditions assumed (variation only with z, and no explicit dependence of f on z), we shall show that for any solution with $\alpha_1''(z_1)$, $\alpha_2''(z_1)$, $\alpha_1''(z_2)$, and $\alpha_2''(z_2)$ not all zero, a variation $\delta\alpha_1(z)$, $\delta\alpha_2(z)$ can be found that makes the second variation of G negative.

For this purpose we consider a variation of the form

$$\delta\alpha_i=\epsilon_1 u_i(z)+\epsilon_2 v_i(z), \quad (11)$$

where ϵ_1 and ϵ_2 are arbitrary small constants. The variation of G, to the second order in ϵ_1 and ϵ_2, is

$$\delta G=\tfrac{1}{2}\{A_{11}[u]\epsilon_1^2+2A_{12}[u,v]\epsilon_1\epsilon_2+A_{22}[v]\epsilon_2^2\}, \quad (12)$$

where A_{11} is a functional of u_1 and u_2, A_{22} of v_1 and v_2, and A_{12} of u_1, u_2, v_1, and v_2. Our proof consists in the construction of a particular $u_1(z)$ and $u_2(z)$ such that $A_{11}=0$ and such that, for suitably chosen $v_1(z)$ and $v_2(z)$, $A_{12}\neq 0$. Then by the calculus of extrema in two independent variables, an ϵ_1 and ϵ_2 can be found for which δG is negative.

The following reasoning leads naturally to a suitable choice of u_i.

To compute the term $A_{12}[u,v]\epsilon_1\epsilon_2$ in Eq. (12), for any u_i and v_i, we can make a variation $\epsilon_1 u_i$ from equilibrium and then make a further variation $\epsilon_2 v_i$ from the already varied state. The first step, to the first order in ϵ_1, produces no change in G. The second step produces a change which, to the first order in ϵ_2, is given by Eq. (7) with $\delta\alpha_i$ set equal to $\epsilon_2 v_i$ and with the coefficients of $\delta\alpha_i$ evaluated at the end of the first step. If these coefficients are now evaluated only to the first order in ϵ_1, the result neglects the part of δG proportional to ϵ_1^2, as well as the part proportional to ϵ_2^2 and already neglected, but evaluates correctly the part proportional to $\epsilon_1\epsilon_2$ and therefore enables us to evaluate $A_{12}[u,v]$.

To evaluate $A_{11}[u]$, we note that the formula for $A_{12}[u,v]$ holds for any v_i and therefore, in particular, for $v_i=u_i$. But setting $v_i=u_i$ in Eq. (11) is equivalent to replacing ϵ_1 by $\epsilon_1+\epsilon_2$ and v_i by 0. Therefore $A_{11}[u]\epsilon_1^2+2A_{12}[u,u]\epsilon_1\epsilon_2+A_{22}[u]\epsilon_2^2$ must be equal to $A_{11}[u](\epsilon_1+\epsilon_2)^2$ for arbitrary ϵ_1 and ϵ_2, whence $A_{11}[u]=A_{12}[u,u]$. We can therefore find $A_{11}[u]$ by replacing v_i by u_i in the formula for $A_{12}[u,v]$.

Now consider a variation $\epsilon_1 u_i$ that consists in a shift of the equilibrium solution along Oz by a distance $-\epsilon_1$; that is,[5] $\epsilon_1 u_i=\alpha_i(z+\epsilon_1)-\alpha_i(z)$ or, to the first order in ϵ_1,

[5] The values of $\alpha_i(z+\epsilon_1)$ at points z such that $z+\epsilon_1$ is outside the specimen correspond to continuations of the motion of the analogous particle, under the same conservative forces, to times z earlier than z_1 or later than z_2.

$u_i=\alpha_i'$. The varied functions $\alpha_i(z+\epsilon_1)$ satisfy the differential equations (8) exactly, but they fail to satisfy the boundary conditions (9) by an error of order ϵ_1; therefore the change δG due to the second step $\epsilon_2 v_i$ receives no contribution from the integral in (7) but only contributions from the boundary terms. In the special case $v_i=u_i=\alpha_i'$, the boundary terms also vanish, so that $A_{11}[u]=0$. To show that $A_{12}[u,v]$ can be made to differ from 0, we write δG explicitly:

$$\delta G=[(m_{11}\alpha_1'+m_{12}\alpha_2')\epsilon_2 v_1+(m_{12}\alpha_1'+m_{22}\alpha_2')\epsilon_2 v_2]\Big|_{z_1+\epsilon_1}^{z_2+\epsilon_1}$$
$$=\epsilon_1\epsilon_2[(m_{11}\alpha_1''+m_{12}\alpha_2'')v_1+(m_{12}\alpha_1''+m_{22}\alpha_2'')v_2]\Big|_{z_1}^{z_2}, \quad (13)$$

since the terms $\epsilon_1\epsilon_2(\partial m_{ij}/\partial\alpha_k)v_i\alpha_j'\alpha_k'$ vanish at the boundaries. Now suppose that either α_1'' or $\alpha_2''\neq 0$ at z_2: we can take, for example, $v_i(z_1)=0$, $v_i(z_2)=\alpha_i''$; then by virtue of the positive definiteness of (m_{ij}), the right member of Eq. (13) will be nonzero. Therefore, A_{12} in Eq. (12) can be made nonzero by proper choice of v_i.

We now give a formal proof, not dependent on the devious reasoning used above for evaluating $A_{12}[u,v]$ and $A_{11}[u]$. We take $u_i=\alpha_i'$. Let

$$x_1=\alpha_1', \quad x_2=\alpha_2', \quad x_3=\alpha_1, \quad x_4=\alpha_2; \quad (14)$$

write L_i for $\partial L/\partial x_i$, L_{ij} for $\partial^2 L/\partial x_i\partial x_j$; and let q' represent dq/dz for any quantity q. Then direct expansion to the second order in the variations

$$\delta x_i=\epsilon_1 x_i'+\epsilon_2 w_i, \quad (15)$$

(where $w_1=v_1'$, $w_2=v_2'$, $w_3=v_1$, $w_4=v_2$) gives Eq. (12), with, for example,

$$A_{12}[u,v]=\int_{z_1}^{z_2}\sum_{i=1}^{4}\sum_{j=1}^{4}L_{ij}x_i'w_j\,dz$$
$$=\int_{z_1}^{z_2}\sum_{j=1}^{4}w_j\{\sum_{i=1}^{4}L_{ij}x_i'\}dz$$
$$=\int_{z_1}^{z_2}\sum_{j=1}^{4}w_jL_j'\,dz. \quad (16)$$

But from the differential equations (8),

$$L_1'=L_3, \quad L_2'=L_4; \quad (17)$$

and from the definitions,

$$w_1=w_3', \quad w_2=w_4'. \quad (18)$$

Hence

$$A_{12}[u,v]=\int_{z_1}^{z_2}(w_3'L_3+w_4'L_4+w_3L_3'+w_4L_4')dz$$
$$=(w_3L_3+w_4L_4)\Big|_{z_1}^{z_2}=\left(v_1\frac{\partial L}{\partial\alpha_1}+v_2\frac{\partial L}{\partial\alpha_2}\right)\Big|_{z_1}^{z_2}, \quad (19)$$

which is equivalent to Eq. (13) by virtue of Eq. (8) (applied at a boundary point) and Eq. (10). A similar calculation with v_i replaced by α_i' shows that $A_{11}[u]=0$. The proof that $A_{12}[u,v]$ can be made different from zero is the same as before.

4. APPLICATION

The theorem thus proved rules out, as unstable, all non-uniform strictly one-dimensional equilibrium states in a homogeneous specimen. Two types of nonuniform one-dimensional state remain physically significant.

First, suppose that there is still variation only with z but that the material is not homogeneous, i.e., that the parameters in f vary with z. (This includes, as a limiting case, surface anisotropy.) We may regard an inhomogeneous specimen as an originally homogeneous one perturbed by a nonuniformity of properties. If the perturbation is small, states derived from stable uniform states will be stable, and all other states will be unstable. As the perturbation increases, it may destabilize some states and stabilize others; the number of stable states need not be conserved in the process. Thus our theorem does not invalidate Aharoni's calculations[6] on the effect of imperfections; the stability of his states must be investigated directly.

Second, consider the Landau-Lifshitz method[7,8] of calculating the internal structure and energy of a Bloch wall. Here the boundary conditions are imposed in advance: the magnetization is required to have a specified direction at $z=-\infty$ and another at $z=+\infty$. The stability of at least one nonuniform solution is thereby assured. But no grounds for imposing such boundary conditions will be found in any strictly one-dimensional situation; they come out of a previous three-dimensional analysis on a larger scale, with exchange energy neglected and discontinuities of magnetization therefore allowed. Such discontinuities, as in the familiar "closure-domain" model, minimize the magnetostatic energy; the wall calculation is then a method of patching up the model by replacing discontinuities by gradual transitions. The wall calculation, therefore, derives its justification from three-dimensional considerations implicit in the initial statement of the formally one-dimensional problem.

In calculations such as those of Kaczér,[9] the boundary conditions imposed are not that the magnetization have specified directions at $z=\pm\infty$ but that its direction cosines be periodic, with a specified period. The justification for the periodic boundary conditions and for the exclusion of the uniform solution must come from three-dimensional considerations similar to those that justify the Landau-Lifshitz calculation.

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The three-dimensional considerations implicit in wall calculations are seldom mentioned. In fact, it is usual to assume that a minimum of G has been found when, in fact, all that has been found is a solution of the Euler equations (8). Nothing is said about the substitution of another boundary condition for the one that comes, just as unambiguously as does the differential equation, out of the formal variational procedure; and nothing is said about the sign of the second variation, which determines the stability. It does not follow from this that the usual calculations are necessarily not useful, but it does follow that they are lacking in completeness and consistency.

Finally, let us examine, from a three-dimensional point of view, a uniform state that was found stable under the constraint of one-dimensionality. If the magnetization has no component along Oz, the state is stable with respect to arbitrary three-dimensional variations; for every term in G is at a minimum with respect to such variations. But if there is a z component, removal of the constraint may allow a decrease of G by development of a structure nonuniform in x and y; for such nonuniformity can decrease the magnetostatic energy. Thus domain formation appears to be an essentially two- or three-dimensional phenomenon.

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Hardness of Nonmetallic Solids on an Atomic Basis

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Hardness values of 65 nonmetallic crystalline solids of 16 different structures are compared with data of a newly introduced concept: "the volumetric lattice energy." When such solids are classified according to a new interpretation of lattice anharmonicity, a set of linear interrelations is obtained which covers the entire hardness range. Thus, on the basis of interatomic cohesive forces, the over-all hardness of these solids becomes unambiguously defined. Hardness receives the dimension (ergs/cm^3) or (kcal/cm^3), and an absolute scale. Such hardness data become independent of anisotropy, structure type, and valency of the atoms. Conversion from relative to absolute hardness, as well as estimation of lattice energy data through appropriate hardness testing, becomes possible. For example, the extremely high hardness value of the rare type-II diamond could be determined to be 1.7 times that of the type-I diamond, purely from atomic data. Analogous treatment of the hardness of metallic solids poses additional problems.

I. INTRODUCTION

ALL hardness measurements are relative, and the data obtained by the many different methods of hardness testing are for the greater part not comparable with one another.[1] The hardness of a solid is defined by the resistance against lattice destruction and is considered to be a function of the interatomic forces.[2] Attempts towards a physical definition of hardness were made by Friedrich, Goldschmidt and others.[3] Yet hardness has in general defied unambiguous physical definition.[4] This presentation intends to develop such a definition.

The vast majority of hardness data of crystals are given in numerical units according to Mohs (M scale). Therefore, the experimental hardness data of this study for the greater part refer to this M scale. As recent work shows, there is a sound physical basis upon which equal intervals of scratch-hardness can be constructed and, in fact, the M scale follows it surprisingly well up to the relative hardness $H=9$.[5] About 99% of all known materials belong to a hardness range from $H=1$ to $H=9$, while the relative difference in hardness between successive materials is small within this range. Thus the M scale is quantitatively useful up to $H=9$.

However, the complementary range between corundum and diamond (corresponding to $H=9$ and 10 in

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