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Generalized self-consistency test of wall computations

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The criterion for checking the self-consistency of magnetic domain wall computations, which has been used before for several particular cases, is generalized for walls with a non-zero applied field. Other criteria are established for one-dimensional domain walls, and many examples are given for the usefulness of these criteria.

I. INTRODUCTION

In a preliminary report[1] we have proved that, *at an energy minimum*, the domain wall energy density,

$$w_{\text{wall}}=w_e+w_a+w_m+w_f, \tag{1}$$

must be equal to

$$w'_{\text{wall}}=w'_e+w'_a+w'_m+w'_f. \tag{2}$$

Here w_e, w_m, w_a and w_f are the exchange, magnetostatic, anisotropy, and external field energy densities respectively in the wall, as separated from the effect of the domains on both sides of the wall. The general method for evaluating the primed energy densities in Eq. (2) was outlined in Ref. 1, but the specific expression given for w'_a in one-dimensional walls applies only to the case of zero applied field. The proof given there (which will be generalized here) for the equivalence of the expressions in Eqs. (1) and (2) at the energy minima actually applies to the **energy densities** at every point of the wall, and not only to the integrated, total energies. However, for a criterion for the validity of the computations, it is not practical to check every point, and one should be satisfied with a test that applies to the average.

It has already been demonstrated in several studies that the closeness to 1 of the ratio (formerly denoted by S) of the *integrated* expressions in Eqs. (1) and (2),

$$S_0=\gamma_{\text{wall}}/\gamma'_{\text{wall}}, \tag{3}$$

can serve[1–6] as a quantitative measure of the closeness of the computed wall structure to the true minimal energy state. This self-consistency parameter, S_0, is defined here with the subscript 0, to distinguish it from other such parameters[7] which will be discussed in the following Sec. IV. Numerical examples for the closeness of S_0 to 1 in properly minimized wall structures were given[1] for zero applied field only. Some *two-dimensional* wall structures were also reported by Yuan and Bertram[5] for a moving wall, in a non-zero applied field. However, they[5] tabulated the value of this parameter, S_0, only for the case of a zero applied field, because they did not have its definition for the other cases they studied. This definition will be extended in the next section to include the case of a non-zero applied field, but only for a stationary wall. We will prove in that section the equivalence of the expressions in Eqs. (1) and (2) at the energy minima for this generalized case, and will give specific expressions for the energy density terms in these relations. The *numerical* results in Sec. V of this paper will be restricted to one-dimensional walls, both for the sake of simplicity, *and* because one-dimensional walls have other, independent self-consistency tests. Some of the examples may be so simple that their energy minimization does not really need any independent tests. Such cases serve more as an illustration for the validity of the present criteria than as a check on the validity of the computations.

II. THEORY

Consider a homogeneous ferromagnetic slab, $-b \leqslant y \leqslant b$, which is infinite along x and z. The regions $|x| \geqslant a$ are assumed to be two domains, which are uniformly magnetized in directions that need not be specified at this stage. The domain wall is the region $|x| \leqslant a$, or *part* of it, because a part of that region may also belong to the domains and not to the wall. Therefore, this definition includes *in principle* subdivided Bloch walls, which are observed[8] even in bulk Fe, as well as cross-tie walls,[9] even though these cases will not be specifically addressed in the following.

A wall that extends to infinity along z must have a *periodic* structure in that direction. We denote this periodicity by $2c$, and assume that the direction cosines α, β and γ of the magnetization vector $\mathbf{M}$ and their derivatives at $z=c$ have the same values as at $z=-c$. This periodicity will not be specifically used in the following, because we will use the energy *densities*. It should just be borne in mind that the general case is where the energy per unit wall area is obtained from integrals of the form

$$\gamma_{\text{wall}}=\frac{1}{4bc}\int_{-c}^{c}\int_{-b}^{b}\int_{-a}^{a} w_{\text{wall}}\,dx\,dy\,dz. \tag{4}$$

Only in a 180° wall can the magnetostatic energy of the wall be separated from that of the domains. At any other wall angle there is a surface charge on $x=\pm a$, which interacts with the magnetization. Moreover, an applied magnetic field may affect the magnetization in the *domains*, and not only in the wall separating them, thus modifying this surface charge. To separate the effect of the charge from the study of the wall itself, we cancel this surface charge by subtracting a constant magnetization vector, as has been done[7] for the particular case of a 90° domain wall.

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We thus define V as the potential of the volume and surface charge of $\mathbf{M} - M_s\Theta\mathbf{i}$, where M_s is the saturation magnetization, and Θ is determined by the surface charge on $x=\pm a$. In the case of zero applied field, the parameter Θ was[1] just a constant, which could be defined as a particular number for each particular one-dimensional wall. In the more general case, this Θ must be made equal to the value of the direction cosine α *in the domains*, which needs to be evaluated for every case, and which depends on the applied field. More than one wall may also be included in principle in this study. For example, in the case of two parallel 180° walls in a field applied in the z-direction[10] the appropriate value is $\Theta=0$, because there is no charge on $x=\pm a$. For the one-dimensional walls, we define $\Theta_0 = 0, 1/\sqrt{3}, 1/\sqrt{2}$ and $\sqrt{2/3}$ for 180°, 109°, 90° and 71° walls respectively, and use the notation

$$\Theta_d=\Theta-\Theta_0. \tag{5}$$

Under these assumptions, the magnetostatic energy density is

$$w_m=\tfrac{1}{2}M_s[(\alpha-\Theta)\partial V/\partial x+\beta\partial V/\partial y+\gamma\partial V/\partial z]. \tag{6}$$

The exchange energy density is

$$w_e=\tfrac{1}{2}C[(\nabla\alpha)^2+(\nabla\beta)^2+(\nabla\gamma)^2], \tag{7}$$

where C is the exchange constant. The anisotropy energy density will not be specified at this stage, and will just be written as the term w_a. We also consider an applied field, $\mathbf{H}$, and take the energy density of its interaction with the magnetization as

$$w_f=-\mathbf{M}\cdot\mathbf{H}. \tag{8}$$

When the total wall *energy*,

$$\gamma_{\text{wall}}=\gamma_e+\gamma_m+\gamma_a+\gamma_f, \tag{9}$$

is minimized for all possible magnetization configurations, the following differential equations are obtained:

$$C[\nabla^2\alpha-(\alpha/\gamma)\nabla^2\gamma]-\partial w_a/\partial\alpha$$
$$+M_s[H_x-\partial V/\partial x-(\alpha/\gamma)(H_z-\partial V/\partial z)]=0, \tag{10}$$

and

$$C[\nabla^2\beta-(\beta/\gamma)\nabla^2\gamma]-\partial w_a/\partial\beta$$
$$+M_s[H_y-\partial V/\partial y-(\beta/\gamma)(H_z-\partial V/\partial z)]=0, \tag{11}$$

with the boundary conditions

$$\partial\alpha/\partial y=\partial\beta/\partial y=\partial\gamma/\partial y=0 \quad \text{at} \quad y=\pm b, \tag{12}$$

besides the requirement of periodicity in z, and besides some boundary conditions at $x=\pm a$, which need not be specified explicitly for the present purpose.

When Eq. (10) is multiplied by $\alpha-\Theta$ and Eq. (11) by β, and they are added together, simple transformations of the various terms, with the use of the identity

$$\alpha^2+\beta^2+\gamma^2=1, \tag{13}$$

leads to some of the energy *density* expressions in the foregoing. In the previous derivation[1] we have integrated the energy densities, but it turns out that this step is not necessary. In particular, the transformation of the terms with ∇^2 to the form of the exchange energy term of Eq. (7) can be done without an integration, under the *only* assumption that Eq. (13) is fulfilled. The end result is that the energy *density* of Eq. (1) is identical to that of Eq. (2), where the latter can be written specifically as

$$w'_{\text{wall}}=w'_a+w'_f-\tfrac{1}{2}\Theta C\nabla^2\alpha+(1/2\gamma)$$
$$\times(1-\alpha\Theta)[M_s(\partial V/\partial z)-C\nabla^2\gamma], \tag{14}$$

with

$$w'_f=-\frac{M_s}{2}\left[(\alpha+\Theta)H_x+\beta H_y+\left(\gamma+\frac{1-\alpha\Theta}{\gamma}\right)H_z\right] \tag{15}$$

and

$$w'_a/K=\beta^2[c_1\beta^2+c_2\alpha(\alpha-\Theta_0)]-c_3(\alpha-\Theta_0)^3(\alpha+\Theta_0)$$
$$+\alpha\Theta_d[2c_3(\alpha-\Theta_0)(\alpha+\Theta_0)-c_2\beta^2+c_4], \tag{16}$$

where $K=|K_c|$ (with $K_c>0$ for 180° walls), $c_1=1,1,\frac{3}{4}$ and $-\frac{3}{4}$, $c_2=1,1,-1$ and $-\frac{5}{2}$, $c_3=-1,\frac{3}{4},1$ and $-\frac{3}{4}$, $c_4=1,0,0$ and 0, for 180°, 109°, 90° and 71° walls respectively.

This equivalence of the primed and unprimed energy densities is for α, β and γ which fulfill the differential equations, Eq. (10) and Eq. (11), which must be fulfilled at an energy minimum. Therefore, a *necessary* condition for the computed structure to be close to a true minimum energy state is that the expression in Eq. (14) is approximately equal to that in Eq. (1), at each point in the wall. However, since it is not practical to check every point, it is better to check the average (or integrated) values, and demand that the ratio in Eq. (3) is approximately 1. The term with $\nabla^2\alpha$ in Eq. (14) is expected to vanish when integrated, because of the boundary conditions. It is only included here to emphasize the derivation of this equation.

The same proof for the equality of Eqs. (1) and (2) in the wall applies also to the energy terms in the domains. However, in the uniformly-magnetized domains there is no contribution from the exchange energy, and if there is a demagnetizing field (in films of finite thickness), it is uniform. We may thus take $w'_e=0$, and the equivalence of the energy densities becomes

$$w_a+w_m+w_f=w'_a+w'_f, \tag{17}$$

where

$$w_m=2\pi pM_s^2\beta^2, \tag{18}$$

and $p=1$ for films of finite thickness and $p=0$ for infinite media. The expressions for the primed energy densities in the domains are the same as those in the wall.

In order to separate the domain energy from the wall energy, we add a constant to each of the energy density terms. Specifically, we define

$$\epsilon_a=w_a-C_a, \quad \epsilon_m=w_m-C_m, \quad \epsilon_f=w_f-C_f, \tag{19a}$$

$$\epsilon'_a=w'_a-C'_a, \quad \epsilon'_f=w'_f-C'_f, \tag{19b}$$

where four of the five constants, C_a, C_m, C_f, C'_a and C'_f are arbitrary, while the fifth one is determined by the relation

$$C_a+C_m+C_f=C'_a+C'_f, \tag{20}$$

which results from Eq. (17). We choose these arbitrary constants so that they make ϵ_a, ϵ_m, ϵ_f, ϵ'_a and ϵ'_f vanish in the domains. Specifically, we have

$$C_a=w_a(\alpha_0,\beta_0), \tag{21a}$$

$$C_m=2\pi pM_s^2\beta_0^2, \tag{21b}$$

$$C_f=-M_s(\alpha_0H_x+\beta_0H_y+\gamma_0H_z), \tag{21c}$$

$$C'_a=C_a+C_m-\frac{1}{2}M_s\left((\alpha_0-\Theta)H_x+\beta_0H_y - \frac{\alpha_0(\alpha_0-\Theta)+\beta_0^2}{\gamma_0}H_z\right), \tag{21d}$$

and

$$C'_f=-\frac{1}{2}M_s\left[(\alpha_0+\Theta)H_x+\beta_0H_y + \left(\gamma_0+\frac{1-\alpha_0\Theta}{\gamma_0}\right)H_z\right], \tag{21e}$$

where α_0 and β_0 are the values of the direction cosines α and β in the domains.

For the calculation of α_0, β_0 and γ_0 separate equations can be derived for many particular cases, as Hubert did for example[4] for his model of a certain one-dimensional wall, in a non-zero applied field. Some such cases will be given in full in the following section. Here we describe a more general method, which works for *all* cases, and which may sometimes be more convenient to use than the special solutions for the particular cases.

Following LaBonte[3] we differentiate the total wall energy density, Eq. (1), with respect to all three direction cosines, and apply the constraint of Eq. (13) to find the constrained minimum conditions

$$\alpha=-\frac{1}{R}\left(\frac{\partial w}{\partial\alpha}\right)_{\beta,\gamma}, \quad \beta=\frac{1}{R}\left(\frac{\partial w}{\partial\beta}\right)_{\gamma,\alpha}, \tag{22a}$$

and

$$\gamma=-\frac{1}{R}\left(\frac{\partial w}{\partial\gamma}\right)_{\alpha,\beta}, \tag{22b}$$

where we use w for w_{wall}, and where

$$\left(\frac{\partial w}{\partial\alpha}\right)_{\beta,\gamma}=-\left(\frac{\partial w_u}{\partial\alpha}\right)_{\beta,\gamma}+M_sH_x, \tag{23a}$$

$$\left(\frac{\partial w}{\partial\beta}\right)_{\gamma,\alpha}=-\left(\frac{\partial w_a}{\partial\beta}\right)_{\gamma,\alpha}-4\pi pM_s^2\beta+M_sH_y, \tag{23b}$$

$$\left(\frac{\partial w}{\partial\gamma}\right)_{\alpha,\beta}=-\left(\frac{\partial w_a}{\partial\gamma}\right)_{\alpha,\beta}+M_sH_z, \tag{23c}$$

and

$$R=\sqrt{\left(\frac{\partial w}{\partial\alpha}\right)_{\beta,\gamma}^2+\left(\frac{\partial w}{\partial\beta}\right)_{\gamma,\alpha}^2+\left(\frac{\partial w}{\partial\gamma}\right)_{\alpha,\beta}^2}. \tag{23d}$$

Using suitable starting values for α, β and γ, these equations can be used to obtain successively better approximations to α_0, β_0 and γ_0.

III. SPECIFIC CASES

For a one-dimensional wall, in an infinite medium, $p=0$ in Eq. (18), so that $w_m=0$. Therefore, only four of the five constants mentioned in the previous section exist in this case. Specific expressions for these four parameters, and for α_0, β_0 and γ_0, are given here for some one-dimensional walls, for which the conditions for an energy minimum can be solved in a closed form.

(1) For 180° walls in a uniaxial-anisotropy material, in a field applied perpendicular to the z-axis, we have

$$w_a=K_u(\alpha^2+\beta^2), \tag{24a}$$

$$w_f=-H_xM_s\alpha-H_yM_s\beta. \tag{24b}$$

The equilibrium direction cosines are

$$\alpha_0=\frac{H_xM_s}{2K_u}, \quad \beta_0=\frac{H_yM_s}{2K_u}. \tag{24c}$$

We also have

$$w'_a=K_u\alpha\alpha_0. \tag{24d}$$

The four constants are then

$$C_a=\frac{M_s^2}{4K_u}(H_x^2+H_y^2), \quad C_f=-\frac{M_s^2}{2K_u}(H_x^2+H_y^2), \tag{25a}$$

$$C'_a=\frac{H_x^2}{4K_u}, \quad C'_f=-\frac{M_s^2}{4K_u}(2H_x^2+H_y^2). \tag{25b}$$

(2) For 180° walls in a material with both uniaxial and cubic anisotropy,

$$\partial w_a/\partial\alpha=2\alpha[K_u+K_c(1-2\alpha^2-\beta^2)], \tag{26a}$$

$$\partial w_a/\partial\beta=2\beta[K_u+K_c(1-\alpha^2-2\beta^2)]. \tag{26b}$$

If $H_y=0$, $\beta=0$; α_0 is the solution of

$$4K_c\alpha_0^3-2(K_u+K_c)\alpha_0+M_sH_x=0. \tag{27}$$

If $H_x=0$, $\alpha=0$; β_0 is the solution of

$$4K_c\beta_0^3-2(K_u+K_c)\beta_0+M_sH_y=0. \tag{28}$$

(3) For 90° walls with cubic anisotropy,

$$\partial w_a/\partial\alpha=2K_c\alpha(2\alpha^2+\beta^2-1), \tag{29a}$$

$$\partial w_a/\partial\beta=K_c\beta(2\alpha^2-3\beta^2+1). \tag{29b}$$

If $H_y=0$, $\beta=0$; α_0 is the solution of

$$4K_c\alpha_0^3-2K_c\alpha_0-M_sH_x=0. \tag{30}$$

If $H_x=0$, $\alpha\neq0$;

$$\alpha^2=\tfrac{1}{3}(1-\beta^2); \tag{31}$$

hence, β_0 is the solution of

$$4K_c\beta_0^3-2K_c\beta_0+M_sH_y=0. \tag{32}$$

(4) For 71° walls with cubic anisotropy,

$$\partial w_a/\partial \alpha = K_c \alpha(3\alpha^2+5\beta^2-2), \tag{33a}$$

$$\partial w_a/\partial \beta = K_c \beta(5\alpha^2+3\beta^2-2). \tag{33b}$$

If $H_y = 0$, $\beta=0$; α_0 is the solution of

$$3K_c \alpha_0^3 - 2K_c \alpha_0 - M_s H_x = 0. \tag{34}$$

If $H_x = 0$, $\alpha \neq 0$;

$$\alpha^2 = \tfrac{1}{3}(2-5\beta^2). \tag{35}$$

Hence, β_0 is the solution of

$$16K_c \beta_0^3 - 4K_c \beta + 3M_s H_y = 0. \tag{36}$$

IV. ONE-DIMENSIONAL WALLS

Several authors who studied various particular cases of one-dimensional micromagnetics have been able to integrate Brown's differential equation once for those cases, thus reducing it from a second order equation to a first order one. These cases were reviewed and expressed in a more general form.[11] In a slightly different notation, Eq. (26) of Ref. 11 means that the expression

$$A^* = w_e - w_m - w_a - w_f, \tag{37}$$

has been proved to be a first integral in any one-dimensional micromagnetics problem. In other words, this A^* is a constant, which has the same value for every value of x. With a proper choice of the boundary conditions (or the zero energy level) this constant can be taken as zero, so that one of the energy density expressions can be obtained from the others, if the magnetization configuration is a solution of Brown's equation, i.e., if the wall energy is properly minimized. As a check of the accuracy of numerical computations of the different energy terms, we use again only the average, namely the integral over x, and define a self-consistency parameter[12] as:

$$S_1 = (\gamma_e - \gamma_m - \gamma_a - \gamma_f)/\gamma_{\text{wall}}, \tag{38}$$

where the γ-s are the energy terms corresponding to the w-s. A good minimization must have $|S_1| \ll 1$, as was the case in some examples reported before,[12] and in other examples to be given here.

It should be noted that the argument concerning this parameter S_1, as well as those about the parameter S_2 described in the following, and the parameter S_0 described in the foregoing, are all based on the assumption that the magnetization configuration is a solution of a certain set of differential equations. This assumption breaks down when there is a discontinuity, and it is not clear *a priori* if any of these self-consistency criteria apply for a discontinuous anisotropy, for example. For 71° and 109° walls we[12] have simulated the effect of magnetostriction by including an *additional* anisotropy parallel to the magnetization in each domain, so that its easy axis rotates abruptly at the center of the wall. For that case we found that S_1 was very small for a properly minimized wall. However, neither S_0 nor S_2 was close to 1 for these walls.

A third criterion is also possible, but only in one dimension. In order to derive it, we first note that the choice in Sec. II, of multiplying Eq. (10) by $\alpha-\Theta$ and Eq. (11) by β (before they are added together) is arbitrary. It is possible to use a different linear combination, and in particular to multiply Eq. (10) by $\alpha - c$, instead of $\alpha-\Theta$, and add it to Eq. (11) multiplied by β. For any choice of this arbitrary constant, c, the transformations are rather similar to the previous case, and can lead to *another* self-consistency test. Yet in most cases this latter test is not practical, because the magnetostatic energy will contain a term which is proportional to $(c - \Theta)\partial V/\partial x$, and this term decreases very slowly with increasing $|x|$. Moreover, it carries over into the domains, and mathematically it becomes 0 only at infinity. In practice there is not even any finite distance within the domain from which one can approximate the integrated contribution of this term by a *constant*, and corrections such as those in section II cannot work unless one is ready to go up to impractically large values of x. Cases like this one have been encountered before[13] when equally legitimate self-consistency tests were exploded by a term that formally tended to infinity.

The obvious solution is to eliminate this troublesome term by choosing $c = \Theta$, as we did in the foregoing. But there is also one case in which any other value of c may be chosen. In one dimension (and *only* in one dimension) the above-mentioned term is proportional to the x-component of the magnetization, leading to strictly local variation with no interaction from the other part. In this case the contribution in the domains is 0, and the magnetostatic term behaves in the same way as other terms. Therefore, when the wall is one dimensional, i.e., when the magnetization is a function of x only, there is an extra, and independent, self-consistency parameter,

$$S_2 = \gamma_{\text{wall}}/\gamma''_{\text{wall}}, \tag{39}$$

which should also be nearly 1 when the energy is properly minimized. Here

$$\gamma''_{\text{wall}} = -\frac{1}{2}\int_{-a}^{a} \left\{ \frac{C}{\gamma}\frac{d^2\gamma}{dx^2} + \alpha\frac{\partial w_a}{\partial \alpha} + \beta\frac{\partial w_a}{\partial \beta} - 2w_a + M_s\left[\alpha H_x + \beta H_y + \left(\gamma + \frac{1}{\gamma}\right)H_z\right] + 4\pi M_s^2 \Theta(\alpha-\Theta)\right\} dx. \tag{40}$$

A particular case of this expression, for a 90° wall, has already been used in Ref. 7. For a 180° wall $\Theta = 0$ if $H_x = 0$, and in this case the expression in Eq. (40) is identical to that for γ'_{wall} in Ref. 1. Therefore, for this case there is nothing new in S_2, which just coincides with S_0.

V. NUMERICAL RESULTS

All the computations reported here were carried out using essentially the same method as that used by Brown and LaBonte[14] to compute the one-dimensional 180° wall, and which we[1,7,12] used for studying other one-dimensional walls. In all our computations, the wall was subdivided into 801 prisms of width 1.25 nm in the x-direction. All

TABLE I. The self-consistency parameters, S_0, S_1, and S_2, of one-dimensional walls with wall angle ϕ, in an applied field **H** (in Oe), for Fe with an exchange constant $C = 2 \times 10^{-6}$ erg/cm and saturation magnetization $M_s = 1700$ emu. The cubic anisotropy constant, K_c, and the uniaxial anisotropy constant, K_u, are in units of 10^5 erg/cm^3.

K_c	K_u	H_x	H_y	$10^4(1-S_0)$	10^4S_1	$10^4(1-S_2)$
				$\phi=90°$		
4.75	0	280	0	6.13	7.15	32.7
				$\phi=180°$		
0	1.0	0	59	2.50	0.92	2.50
0	1.0	59	0	1.42	1.09	1.91
0	1.0	0	0	1.60	1.49	1.60

computations were carried on until the maximum angle by which the magnetization rotated in one iteration was 2×10^{-8} or less.

Some examples for the effect of an applied field are given in Table I, which lists all the three parameters S_0, S_1 and S_2 in several one-dimensional 90° and 180° walls. In all these walls the parameters of Fe were used, namely an exchange constant $C = 2 \times 10^{-6}$ erg/cm and a saturation magnetization $M_s = 1700$ emu. The 90° wall was computed for a cubic anisotropy constant $K_c = 4.75 \times 10^5$ erg/cm^3, and the 180° walls were computed for a uniaxial anisotropy constant $K_u = 10^5$ erg/cm^{-3}.

Table II lists the parameters S_0 and S_1 in one-dimensional 180° walls, for a material with negative cubic anisotropy constant, $K_c = -4.5 \times 10^4$ erg/cm^3, for different values of the angle ψ between the y axis and the plane containing a third easy axis. These cases were studied analytically by Lilley[15] under the assumption that the magnetostatic energy vanishes, because the differential equation does not have an analytical solution when this energy is included. In some cases this energy is indeed zero, in others Lilley[15] just neglected it. In particular, when this ψ is an integral multiple of 60°, the magnetization rotates through an easy direction, so that the magnetostriction (which we simulate by a uniaxial anisotropy, K_u) is necessary to hold the wall together. In these cases, α vanishes everywhere in the wall, there is no magnetostatic energy, and the computed energy is very close to the analytical value of Ref. 15.

TABLE II. The self-consistency parameters, S_0 and S_1, of a one-dimensional 180° wall for a material with negative cubic anisotropy constant, $K_c = -4.5 \times 10^4$ erg/cm^3, a uniaxial anisotropy constant, $K_u = 4.5 \times 10^3$ erg/cm^3, and with $C = 1 \times 10^{-6}$ erg/cm and $M_s = 550$ emu. Here $S_2 = S_0$.

ψ	$10^5(S_0-1)$	10^5S_1
0	−9.07	9.39
15	0.29	8.68
30	1.60	8.31
45	22.97	8.60
60	9.25	9.32

TABLE III. The self-consistency parameters, S_0, S_1, and S_2, of one-dimensional 90° walls, in zero applied field, for a fictitious material with an exchange constant $C = 2 \times 10^{-6}$ erg/cm and a cubic anisotropy constant $K_c = 4.75 \times 10^5$ erg/cm^3, with a varying saturation magnetization M_s in emu. The total wall energy, $\gamma_{\rm wall}$, and the magnetostatic contribution, γ_m, are also listed, and are in units of erg/cm^2.

M_s	$10^4(1-S_0)$	10^4S_1	$10^4(1-S_2)$	$\gamma_{\rm wall}$	γ_m
1700	1.63	4.33	3.3	1.18	0.60
650	5.04	5.04	11.6	1.14	0.83
340	5.87	4.77	17.6	0.86	0.16
0	4.55	3.21	14.2	0.67	0.00

For other values of ψ, the total energy was slightly decreased by allowing a non-zero value for α, although this value always turned out to be very small. The largest $|\alpha|$ in the entries of Table II was about 2×10^{-4}. The energy difference between the analytical solution (which neglects the magnetostatic term) and our computations was largest for $\psi=30°$, but even for that angle the magnetostatic energy was only 0.2% of the total wall energy. The parameter S_2 is not listed, because it is identical to S_0, as is always the case for one-dimensional 180° walls when no field is applied along x.

Table III lists some results for one-dimensional 90° walls in a fictitious material, with a varying saturation magnetization. This material has the physical parameters of Fe, namely an exchange constant $C = 2 \times 10^{-6}$ erg/cm and a cubic anisotropy constant $K_c = 4.75 \times 10^5$ erg/cm^3. Most of these data have already been published in Ref. 7, including the values of the parameter S_1. The values of S_0 have also been published, in Ref. 1, only they were then called S. These data are repeated here mainly in order to report the values of the third parameter, S_2, and to compare it with the others. Reference 1 also gave some values of S_0 for a *two-dimensional* 90° wall in Fe films. There is no reason to repeat them here.

Computations of 71° and 109° walls have also been reported before[12] and are repeated here (with a few additional cases) mainly in order to include the values of the parameters S_0 and S_2 which were not reported there. These computations were carried out for exchange constant $C = 1 \times 10^{-6}$ erg/cm, cubic anisotropy constant $K_c = -4.5 \times 10^4$ erg/cm^3, and for various values of the saturation magnetization, M_s. For a 109° wall, previous computations[12] simulated the effect of magnetostriction by using an additional uniaxial anisotropy. However, that case, as well as the cases for which this uniaxial anisotropy was added to a 71° wall, yielded values of S_0 and S_2 which were not close to 1, and are, therefore, omitted from the results listed in Table IV . As has already been mentioned in Sec. IV, our criteria cannot be expected to hold for this case of a discontinuity in the easy axis of the anisotropy, even though the S_1 criterion *is* fulfilled there.

Without the additional uniaxial anisotropy, a 109° wall is not stable, but tends to split into two 71° walls. In this work we stabilized it by adding a magnetic field, $H_y = -10$ Oe, instead of stabilizing it by the magnetostriction. This stabilization worked very well, both in the sense that the

TABLE IV. The three self-consistency parameters, S_0, S_1, and S_2, in the normalized form $S_0' = 10^4(1 - S_0)$, $S_1' = 10^4 S_1$, and $S_2' = 10^4(1 - S_2)$, and the values of the direction cosines α and β at the center of the wall, where γ passes through zero, for one-dimensional 71° and 109° walls in a fictitious material with saturation magnetization M_s, in emu. The 109° wall is for an applied field $H_y = -10$ Oe.

M_s	S_0'	S_1'	S_2'	α	β
			71°		
550	1.97	1.67	6.14	.8416	.5402
400	1.34	0.45	4.62	.8665	.4992
350	1.33	0.49	4.87	.8849	.4658
300	1.41	0.72	5.67	.9185	.3953
290	1.54	0.92	6.18	.9289	.3702
280	1.57	0.98	6.49	.9415	.3371
270	1.60	1.05	6.86	.9569	.2904
268	1.82	1.30	7.37	.9605	.2784
265	1.81	1.29	7.44	.9661	.2581
260	1.63	1.12	7.32	.9766	.2151
255	1.65	1.17	7.61	.9887	.1497
253	1.66	1.20	7.74	.9941	.1081
252	1.66	1.21	7.81	.9970	.0776
251	1.68	1.24	7.90	.9998	.0223
250	1.68	1.24	7.87	1.000	1.9×10^{-3}
249	1.67	1.23	7.84	1.000	9.8×10^{-4}
0	1.27	1.68	14.62	1.000	5.6×10^{-7}
			109°		
550	17.49	−0.15	16.78	.5859	.8104

TABLE V. The three self-consistency parameters, S_0, S_1, and S_2, where $S_0' = 10^4(S_0 - 1)$, and the values of the width D of the reversed domain (in nm), for pairs of 180° walls in various applied fields (in Oe), for Fe with an exchange constant $C = 2 \times 10^{-6}$ erg/cm, saturation magnetization $M_s = 1700$ emu, cubic anisotropy constant $K_c = 4.75 \times 10^5$ erg/cm^3, and uniaxial anisotropy constant $K_u = 10^5$ erg/cm^3. In all cases, $H_y = 0$.

H_x	H_z	S_0'	$10^4 S_1$	$10^4\ (S_2-1)$	D
0	1	6.70	3.06	6.70	164.0
0	2	6.70	2.98	6.70	151.7
0	5	7.75	2.84	7.75	133.0
0	10	6.87	2.41	6.87	116.7
0	20	7.89	2.71	7.89	98.93
0	60	7.54	3.40	7.54	70.31
0	100	7.53	4.35	7.53	58.14
0	200	12.3	7.40	12.3	43.80
0	500	2.07	17.2	2.07	29.12
0	700	8.30	23.9	8.30	24.89
0	800	10.6	27.3	10.6	23.36
0	900	9.14	30.7	9.14	22.09
0	1000	5.23	34.1	5.23	21.00
0	1500	−18.8	51.3	−18.8	17.24
0	2000	−38.0	68.9	−38.0	14.96
0	3000	−53.6	105	−53.6	12.21
0	5000	65.0	181	65.0	9.385
0	8000	−141	306	−141	7.300
0	15000	−91.1	689	−91.1	5.056
0	20000	−637	1281	−637	4.047
180	60	5.42	3.12	6.35	101.6

resulting wall was quite similar to the one computed[12] with the additional uniaxial anisotropy, and in the sense of fulfilling all three criteria. The full structure of the wall in this particular case is plotted in Fig. 1 .

The resulting values of the three self-consistency parameters are listed in Table IV. Some idea of the wall structure can be obtained from the values of α and β *at the wall center*, which are also listed in that table. The energy terms are not given here, because they have already been published[12] for most of the entries in the table.

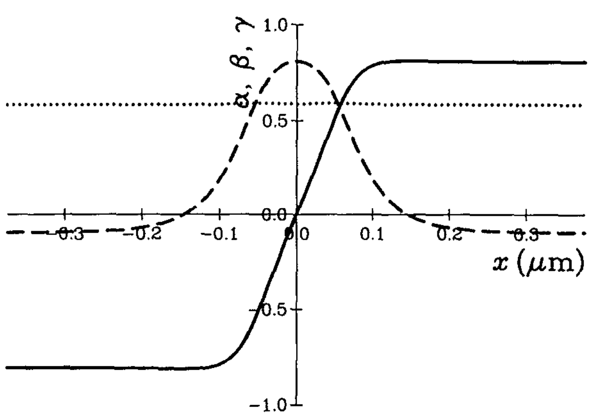

FIG. 1. Magnetization components α (dotted curve), β (dashed curve) and γ (full curve) for a 109° wall in an infinite crystal with $M_s = 550$ emu. Instead of magnetostriction, this particular case is stabilized by a magnetic field $H_y = -10$ Oe.

The effect of a magnetic field with $H_z \neq 0$ on the walls studied in this paper would be to displace them rather than to change their structure. In order to study the effect of such fields on the wall structure, we have considered pairs of walls. The effect of applied fields on pairs of walls in thin films has already been studied.[10] Here we are concerned with one-dimensional walls in an infinite medium. Pairs of one-dimensional 180° Bloch walls may have two possible structures: unwinding or winding, depending on whether the magnetization in the center of the walls is in the same or in opposite directions. Unwinding walls attract each other, and are annihilated in infinitesimally small fields applied parallel to the magnetization in the domains outside the walls. However, winding walls repel each other, and are only annihilated by applied fields large enough to overcome this repulsion. In the present study, we considered pairs of 180° winding walls in iron, with exchange constant $C = 2 \times 10^{-6}$ erg/cm, cubic anisotropy constant $K_c = 4.75 \times 10^5$ erg/cm^3, uniaxial anisotropy constant $K_u = 10^5$ erg/cm^3, and saturation magnetization $M_s = 1700$ emu. A small magnetic field driving the walls towards each other was initially applied, and then gradually increased. The resulting values of the three self-consistency parameters are listed in Table V. The magnetization configuration for a small H_z, and for the largest H_z used, is plotted in Figs. 2 and 3 respectively. Table V also includes one case in which a field with a non-zero x-component was applied. The magnetization in the domains in this case was rotated by 22.28° from the z-direction. This table also shows the width D of the domain between the two walls, which has been calculated as follows:

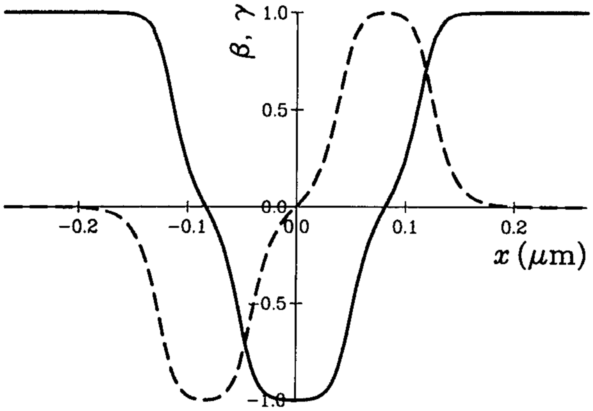

FIG. 2. Magnetization components β (dashed curve) and γ (full curve) for a pair of 180° walls in an infinite crystal, driven towards each other by a magnetic field $H_z = 1$ Oe.

$$D=\frac{1}{2}\int (1-\gamma)dx. \tag{41}$$

It is seen from Table V that S_1 steadily increases with increasing H_z, except for very small fields. It is also seen that S_0 and S_2 (which are identical when $H_x = 0$) do not vary in a regular manner, but remain fairly close to 1 except in very large fields. However, it is seen that in the largest fields applied, D is decreasing towards a value only just over 3 times the subdivision size, which can hardly be considered to be a real double wall, although, as Fig. 3 shows, the appropriate structure is still present. (In fact, this structure is almost identical to that for much lower H_z, except for the change of scale.)

The point is that such high fields are actually much larger than the field needed to saturate the specimen. If the walls are still not annihilated in the computations, it may be because we assume a rigidly one-dimensional structure. It is certainly not clear *a priori* if such an unstable structure, which is not really an energy minimum, is a self-consistent structure, and which, if any, of the criteria should apply. After all, there *is* a lower-energy structure in which these walls annihilate. Therefore, it is particularly interesting to note that these criteria work even for such a case.

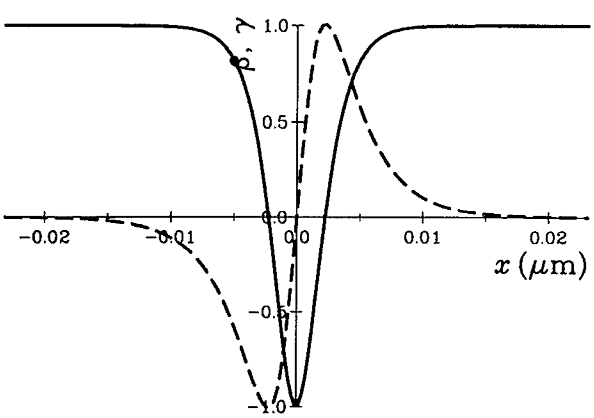

FIG. 3. As Fig. 2, with $H_z = 2 \times 10^4$ Oe.

VI. DISCUSSION

In complicated computations it is always too easy to make programming mistakes, and too difficult to find them. It is, therefore, always helpful to have some criteria for the validity of the results. Such criteria have already been successfully used, and found very useful, in several particular cases of magnetic domain walls. Our generalization of the same criteria should expand their use to other cases. In particular, we give general expressions for the case of an applied magnetic field, which has so far been defined only for a highly-specialized[4] wall model. Yuan and Bertram[5] have already computed some structures of a two-dimensional wall in a non-zero applied field, but reported the values of the self-consistency parameter, S (which is S_0 in the present notation) for zero field only. They may have been able to do better if they had the results presented here, but it should be noted that our study addresses stationary walls only, and does not yet cover the dynamics of a moving wall.

In order to keep this paper to a reasonable size, we have limited the numerical computations to one-dimensional walls. The criteria involving S_1 and S_2 are anyway defined only for one-dimensional walls, and are not valid in two dimensions, as explained in Sec. IV. The criterion that contains S_0 (which was called just S before) has already been reported for many two-dimensional walls in previous publications. Although none of them addressed the case of an applied field, we have not included a numerical example in two dimensions, because they are rather complex, and we consider the one-dimensional examples to be a sufficient illustration of the method. We feel that the separation of the contribution of the domains from that of the wall, which involves complicated computations in two dimensions, could not be clear without these specific examples. Some of the one-dimensional examples involve rather trivial computations, and do not really need a sophisticated check. We consider these cases to be essentially a check of the method itself, namely a test of general expression of Sec. II for these cases. In particular, for the unstable configuration of a double wall, it is certainly not clear *a priori* if these self-consistency tests should apply in the first place.

For the case of one-dimensional walls we report here a rather thorough numerical evaluation for all reasonably conceivable possibilities. We included all the cases for which Lilley[15] gave an analytical solution of the differential equation by neglecting the magnetostatic energy. We minimized the energy for these cases allowing a non-zero magnetostatic energy, and found that the latter was indeed negligibly small. Our result thus justifies the assumption of Lilley[15] and gives a numerical value to the neglected term, which could not be known beforehand. It is not really necessary to apply self-consistency checks to these solutions which are very close to the analytical one, but again we include them as a test of the method itself.

In all these cases we find that all three criteria work very well, in the sense of being fulfilled for a well-minimized wall. They should thus be very useful as routine checks against programming errors, or inadequate minimizing, during all sorts of wall computations. Each of these criteria by itself is only a necessary, and not a sufficient condition. Namely, if it is not fulfilled, the computation is definitely wrong; but if it is fulfilled, the computation cannot be guaranteed to be correct. However, fulfilling all three is highly unlikely to be just fortuitous.

We are giving only a few examples of the actual structures of the walls themselves. Most of the others have been published before, or can easily be extrapolated from the published ones.

Finally, we find it necessary to emphasize again that the whole concept of the self-consistency parameters is based on the assumption that the wall structure under consideration is defined by smooth functions, which are solutions of a certain set of differential equations. A case with any kind of a discontinuity does not necessarily come into this category, but it may just happen to work out anyway. Thus, for the case of a discontinuity in the easy axis of the anisotropy, our criteria cannot be expected to hold, as mentioned in Sec. IV. We find that in this case the S_0 and the S_2 criteria are way off the mark, but the S_1 criterion *is* fulfilled, as listed in Table IV.

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