Vol. A37 (1970) ACTA PHYSICA POLONICA Fasc. 4

MICROMAGNETIC BOUNDARY CONDITIONS IN INHOMOGENEOUS ALLOYS

By F. Goedsche

Department of Physics, Division of Theoretical Physics, Technical University, Dresden*

(Received July 28, 1969)

A system consisting of two ferromagnetic phases is considered. It is assumed that an exchange coupling exists between the phases. A variational procedure is used to derive the boundary conditions at the phase boundary. Micromagnetic equations of motion are associated with these boundary conditions.

1. Introduction

In certain ferromagnetic alloys different magnetic phases can exist side by side (island-structure) [1] whose spatial extension is so big that the application of the macroscopic spin-wave theory is possible for such a system. The magnetic properties of the phases are here characterized by its exchange constants and its spontaneous magnetization. Starting with a microscopic consideration the free enthalpy of a system of two different ferromagnetic phases can be formulated on the fact that an exchange coupling exists between both phases. A variational procedure of the micromagnetism gives the appropriate boundary conditions at this phase boundary.

2. Description of the exchange coupling

The exchange interaction in the considered system shall be described by a Heisenberg-Operator

$$\mathscr{H} = -\frac{1}{2}\sum_{l\neq m} J_{lm}\boldsymbol{S}_l\boldsymbol{S}_m. \tag{1}$$

This expression can be represented by using the magnetization operator

$$\hat{\boldsymbol{M}}(\boldsymbol{r}) = 2\mu_B/\hbar \sum_l \boldsymbol{S}_l\delta(\boldsymbol{r}-\boldsymbol{r}_l) \tag{2}$$

with

$$\mu_B = e\hbar/2mc$$

* Address: Department of Physics, Division of Theoretical Physics, Technical University, Dresden, DDR.

which gives

$$\mathscr{H} = -\frac{1}{2}(\hbar/2\mu_B)^2 \iint d\tau d\tau' J(\boldsymbol{r},\boldsymbol{r}')\hat{\boldsymbol{M}}(\boldsymbol{r})\hat{\boldsymbol{M}}(\boldsymbol{r}'). \tag{3}$$

The exchange interaction is assumed to be short-range. Thus, the exchange integrals $J(\boldsymbol{r},\boldsymbol{r}')$ vanish when $|\boldsymbol{r}-\boldsymbol{r}'|$ exceeds a length of the order of the lattice constant.

To describe especially the interaction of the spins near the boundary between phase 1 and phase 2, we divide the Hamiltonian (3) into the volume term $\mathscr{H}_v$ and the boundary-surface term $\mathscr{H}_B$. Thus

$$\mathscr{H} = \mathscr{H}_v + \mathscr{H}_B \tag{4}$$

with

$$\mathscr{H}_v = -\frac{1}{2}(\hbar/2\mu_B)^2 \iint d\tau d\tau' J_1(\boldsymbol{r},\boldsymbol{r}')\hat{\boldsymbol{M}}_1(\boldsymbol{r})\hat{\boldsymbol{M}}_1(\boldsymbol{r}') \tag{5}$$

and

$$\mathscr{H}_B = -(\hbar/2\mu_B)^2 \iint d\tau d\tau'' J_{12}(\boldsymbol{r},\boldsymbol{r}'')\hat{\boldsymbol{M}}_1(\boldsymbol{r})\hat{\boldsymbol{M}}_2(\boldsymbol{r}'').$$

In this notation $\hat{\boldsymbol{M}}_1$ includes the spin operators of phase 1 and $\hat{\boldsymbol{M}}_2$ the spin operators of phase 2. The integrations of the volume term $\mathscr{H}_v$ cover the whole phase volume. In the boundary-surface term $\mathscr{H}_B$ only the surrounding of the boundary surface contributes to integration because of the short range of the exchange integral J_{12}. To simplify matters the volume term 2 is not considered.

The influence of the boundary-surface term $\mathscr{H}_B$ on the equation of motion of magnetization follows from

$$i\hbar \frac{d}{dt}(\hat{\boldsymbol{M}}_1\boldsymbol{r}_1) = [\hat{\boldsymbol{M}}_1(\boldsymbol{r}_1), \mathscr{H}]. \tag{6}$$

With the familiar commutation relations for the components of magnetization we obtain

$$\begin{aligned}\frac{d}{dt}\hat{\boldsymbol{M}}_1(\boldsymbol{r}_1) &= \hat{\boldsymbol{M}}_1(\boldsymbol{r}_1) \times \frac{\hbar}{2\mu_B}\int d\tau J_1(\boldsymbol{r},\boldsymbol{r}_1)\hat{\boldsymbol{M}}_1(\boldsymbol{r}) \\ &\quad + \hat{\boldsymbol{M}}_1(\boldsymbol{r}_1) \times \frac{\hbar}{2\mu_B}\int d\tau'' J_{12}(\boldsymbol{r}'',\boldsymbol{r}_1)\hat{\boldsymbol{M}}_2(\boldsymbol{r}'').\end{aligned} \tag{7}$$

By the transition from the operators to the macroscopic magnetization $\boldsymbol{M}(\boldsymbol{r}, t)$, assuming cubic symmetry, Eq. (7) yields [2], [3], [4]

$$\begin{aligned}\dot{\boldsymbol{M}}_1(\boldsymbol{r}_1, t) &= \gamma \boldsymbol{M}_1(\boldsymbol{r}_1, t) \times \frac{A_1}{M_1^2}\frac{\partial^2}{\partial \boldsymbol{r}_1^2}\boldsymbol{M}_1(\boldsymbol{r}_1, t) \\ &\quad + \boldsymbol{M}_1(\boldsymbol{r}_1, t) \times \frac{\hbar}{2\mu_B}\int d\tau'' \bar{J}_{12}(\boldsymbol{r}'',\vec{r}_1)\boldsymbol{M}_2(\boldsymbol{r}'', t)\end{aligned} \tag{8}$$

where A_1 is the exchange constant of phase 1; $M_1 = |\boldsymbol{M}_1|$ is the constant magnetization magnitude; and $\gamma = 2\mu_B/\hbar$. The additional term in the micromagnetic equation of motion (8) describes the exchange coupling between both ferromagnetic phases. The properties of the function $\bar{J}_{12}$ indicate that this coupling is significant only near the boundary surface.

A suitable boundary condition should now replace the additional term in Eq. (8). To this end the operator $\mathscr{H}_B$ from Eq. (5) is transformed into a macroscopic energy expression, which is introduced into the free enthalpy of the ferromagnet.

The energy corresponding, in micromagnetic approximation, to the operator $\mathscr{H}_B$ is expressed by

$$E_B = -(\hbar/2\mu_B)^2 \int\int d\tau d\tau'' \bar{J}_{12}(\boldsymbol{r},\boldsymbol{r}'') \boldsymbol{M}_1(\boldsymbol{r}) \boldsymbol{M}_2(\boldsymbol{r}''). \tag{9}$$

The points $\boldsymbol{r}$ and $\boldsymbol{r}''$ are the centroids of small average volumina (containing as usual 30 to 50 elementary cells).

For simplification the following exchange interaction is assumed:

$$\bar{J}_{12}(\boldsymbol{r},\boldsymbol{r}'') = \bar{K}_{12}\, \delta[\boldsymbol{a}+(\boldsymbol{r}-\boldsymbol{r}'')]. \tag{10}$$

Consequently Eq. (9) yields

$$E_B = -(\hbar/2\mu_B)^2 \bar{K}_{12} \int d\tau \boldsymbol{M}_1(\boldsymbol{r}) \boldsymbol{M}_2(\boldsymbol{r}+\boldsymbol{a}). \tag{11}$$

The vector $\boldsymbol{a}$ is to be directed perpendicular to the boundary surface, with $|\boldsymbol{a}|$ in the range of three lattice constants. This corresponds to a nearest-neighbour interaction.

Because the quantities $\boldsymbol{M}(\boldsymbol{r})$ are constant in their average volumes, the expression (11) can be written as a surface integral over the boundary surface F_{12} between both phases. Thus

$$E_B = -K_{12} \int_{F_{12}} df \boldsymbol{M}_1 \boldsymbol{M}_2. \tag{12}$$

In this context, K_{12} is a phenomenological parameter the same as the exchange constants A_1 and A_2.

3. *Variational procedure and boundary conditions*

The free enthalpy of a system consisting of two ferromagnetic phases is (see [3], [4])

$$\begin{aligned} G = {} & \frac{1}{2}\frac{A_1}{M_1^2} \int_{V_1} d\tau \left[\left(\frac{\partial M_1^x}{\partial \boldsymbol{r}}\right)^2 + \left(\frac{\partial M_1^y}{\partial \boldsymbol{r}}\right)^2 + \left(\frac{\partial M_1^z}{\partial \boldsymbol{r}}\right)^2\right] + \int_{V_1} d\tau w_{a_1}(\boldsymbol{M}_1) + \\ & + \frac{1}{2}\frac{A_2}{M_2^2} \int_{V_2} d\tau \left[\left(\frac{\partial M_2^x}{\partial \boldsymbol{r}}\right)^2 + \left(\frac{\partial M_2^y}{\partial \boldsymbol{r}}\right)^2 + \left(\frac{\partial M_2^z}{\partial \boldsymbol{r}}\right)^2\right] + \int_{V_2} d\tau w_{a_2}(\boldsymbol{M}_2) + \\ & + \frac{\mu_0}{2} \int_{\text{space}} d\tau \boldsymbol{H}^2 - A_{12} \int_{F_{12}^{(1)}} df \boldsymbol{M}_1 \boldsymbol{M}_2 - A_{12} \int_{F_{12}^{(2)}} df \boldsymbol{M}_1 \boldsymbol{M}_2 \end{aligned} \tag{13}$$

with the exchange terms particularly valid for cubic symmetry; w_{a_1} and w_{a_2} are the anisotropy-energy densities; and the surface integrals describe the exchange coupling between phase 1 and phase 2. The total field $\boldsymbol{H}$ comprises an applied field and the stray- and the demagnetizing fields.

A special boundary-surface anisotropy is not considered. In equilibrium the free enthalpy G is a minimum, *i.e.* the variation δG vanishes with respect to small deviations of the magnetization. For the calculation of δG rotations of the magnetization only are considered [3]. Thus

$$\delta \boldsymbol{M} = \delta \boldsymbol{\varphi} \times \boldsymbol{M} \text{ with } |\boldsymbol{M}| = \text{const.} \tag{14}$$

Consequently the variation δG is given by [3], [4]

$$\begin{aligned}\delta G = & \int\limits_{V_1} d\tau \left(\boldsymbol{M}_1 \times \left[-\frac{A_1}{M_1^2} \Delta \boldsymbol{M}_1 + \frac{\partial w_{a_1}}{\partial \boldsymbol{M}_1} - (\boldsymbol{H}^a + \boldsymbol{H}_1^d + \boldsymbol{H}_2^s) \right] \right) \delta \boldsymbol{\varphi}_1 + \\ & + \int\limits_{V_2} d\tau \left(\boldsymbol{M}_2 \times \left[-\frac{A_2}{M_2^2} \Delta \boldsymbol{M}_2 + \frac{\partial w_{a_2}}{\partial \boldsymbol{M}_2} - (\boldsymbol{H}^a + \boldsymbol{H}_2^d + \boldsymbol{H}_1^s) \right] \right) \delta \boldsymbol{\varphi}_2 + \\ & + \int\limits_{F_{12}^{(1)}} df \left(\frac{A_1}{M_1^2} \boldsymbol{M}_1 \times \frac{\partial \boldsymbol{M}_1}{\partial n_1} - A_{12} \boldsymbol{M}_1 \times \boldsymbol{M}_2 \right) \delta \boldsymbol{\varphi}_1 + \int\limits_{F_{12}^{(2)}} df \left(\frac{A_2}{M_2^2} \boldsymbol{M}_2 \times \frac{\partial \boldsymbol{M}_2}{\partial n_2} - A_{12} \boldsymbol{M}_2 \times \boldsymbol{M}_1 \right) \delta \boldsymbol{\varphi}_2 = 0\end{aligned} \tag{15}$$

where $\boldsymbol{H}^a$ denotes the applied magnetic field; $\boldsymbol{H}^d$ and $\boldsymbol{H}^s$ the demagnetizing and stray fields and ∂/∂_{n_1}, ∂/∂_{n_2} the derivatives normal to the surfaces $F_{12}^{(1)}$, $F_{12}^{(2)}$ (with $F_{12}^{(1)}, F_{12}^{(2)} \to F_{12}$). Surface terms which do not relate to the boundary surface F_{12} were omitted in Eq. (15).

Because of the arbitrary choice of the variations $\delta \varphi_1$, $\delta \varphi_2$ the preceding expressions must vanish. According to Eq. (15) this gives two differential equations and the associated boundary conditions. For the boundary conditions we obtain

$$\frac{A_1}{M_1^2} \boldsymbol{M}_1 \times \frac{\partial \boldsymbol{M}_1}{\partial n_1} - A_{12} \boldsymbol{M}_1 \times \boldsymbol{M}_2 = 0$$

and

$$\frac{A_2}{M_2^2} \boldsymbol{M}_2 \times \frac{\partial \boldsymbol{M}_2}{\partial n_2} - A_{12} \boldsymbol{M}_2 \times \boldsymbol{M}_1 = 0. \tag{16}$$

The differential equations from (15) are written

$$\boldsymbol{M}_1 \times \boldsymbol{H}_{1\text{eff}} = 0 \text{ and } \boldsymbol{M}_2 \times \boldsymbol{H}_{2\text{eff}} = 0 \tag{17}$$

with

$$\boldsymbol{H}_{\text{eff}} = -\delta G / \delta \boldsymbol{M}.$$

With reference to these equations no boundary conditions exist, which connect magnetization and magnetic fields. Such boundary conditions appear with the magnetostatic potential equations, which must be dealt with when solving Eqs (17).

4. Dynamic equations

The boundary conditions Eq. (16) are also valid for the dynamic modification of Eq. (17), as

$$\dot{\boldsymbol{M}} = \gamma \boldsymbol{M} \times \boldsymbol{H}_{\text{eff}}, \tag{18}$$

which may be derived by means of the Lagrangian formalism [3]

$$\delta \int_{t_1}^{t_2} dtL = 0 \text{ with } L = \int d\tau \mathcal{T}(\boldsymbol{M}, \dot{\boldsymbol{M}}) - G. \tag{19}$$

In comparison with the static case no additional surface integrals emerge here and thus no additional boundary condition. In the simplest form, the consideration of damping leads to the equation of motion written as follows [5]

$$\dot{\boldsymbol{M}} = \gamma \boldsymbol{M} \times [\boldsymbol{H}_{\text{eff}} - \alpha \dot{\boldsymbol{M}}] \tag{20}$$

(α damping constant) which is taken from the more general variational procedure

$$\delta \int_{t_1}^{t_2} dtL - \int_{t_1}^{t_2} dt \int d\tau \frac{\partial \mathcal{F}}{\partial \dot{\boldsymbol{M}}} \delta \boldsymbol{M} = 0 \tag{21}$$

with the dissipation function

$$F = \int d\tau \, \mathcal{F} = \frac{\alpha}{2} \int d\tau \dot{\boldsymbol{M}}^2.$$

This shows that the boundary conditions (16) apply also for the equation of motion with damping.

In the phenomenological description of spin-wave resonances it is frequently possible to consider small deviations from a preferential direction (*e. g.* large applied magnetic field).

Expressing the magnetization with

$$\boldsymbol{M}_1 = M_1 \boldsymbol{l} + \boldsymbol{m}_1 \quad \boldsymbol{M}_2 = M_2 \boldsymbol{l} + \boldsymbol{m}_2 \tag{22}$$

with

$$\boldsymbol{lm} = 0 \text{ and } |\boldsymbol{m}| \ll M$$

($\boldsymbol{l}$ unit vector), with the squared terms in the small quantities $\boldsymbol{m}$ neglected, Eq. (16) yields

$$\frac{A_1}{M_1} \frac{\partial \boldsymbol{m}_1}{\partial n} + A_{12}(M_2 \boldsymbol{m}_2 - M_1 \boldsymbol{m}_2) = 0 \tag{23}$$

and

$$\frac{A_2}{M_2} \frac{\partial \boldsymbol{m}_2}{\partial n_2} A_{12}(M_1 \boldsymbol{m}_2 - M_2 \boldsymbol{m}_1) = 0.$$

Respectively linearized equations of motion are associated with these boundary conditions.

I should like to thank Professor G. Heber and Dr K. Elk for discussions.

REFERENCES

[1] H. Warlimont, H. Mühe, H. Gengnagel, *Z. Angew. Phys.*, **26,** 301 (69); A. Heilmann, W. Zinn *Z. Metallkunde* **58,** 113 (67); H. Wagner, H, Gengnagel, *Phys. Status Solidi* **9,** 45 (65); P. W. Bell-arby, J. Crangle, *J. Appl. Phys.* **39,** 463 (68).
[2] A. I. Achiezer *et al., Spinwellen,* Moskau 1967.
[3] W. F. Brown, *Micromagnetics,* New York, London 1963.
[4] Döring, *Mikromagnetismus, Handbuch der Physik Bd.* 18/2, Berlin, Heidelberg, New York 1966.
[5] T. L. Gilbert, *ARF Project. No.* A 059, Report 1956, (Illinois Institute of Technology).