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Quenching of magnetostriction by torsional strain in zero-magnetostrictive amorphous wire

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Abstract. Simple model band calculations show that torsional stress reduces the absolute value of the Joule magnetostriction λ. This is the consequence of the quenching of orbital magnetism by torsion. The calculations provide an explanation of recent experimental data on almost zero-magnetostrictive amorphous Co-based wire.

1. Introduction

The magnetostriction of metallic wires is of interest from both a technological [1] and a theoretical point of view. In principle, the values of macroscopic magnetoelastic coefficients can be found by means of *ab-initio* band-structure calculations [2]. However, the accuracy of these methods is still too low to expect quantitative results on Joule magnetostriction, and phenomenological approaches are of common use [3, 4] to interpret experimental data.

Recently, the influence of the torsional strain on magnetostriction λ was investigated [5] for $(Co_{95}Fe_5)_{72.5}Si_{12.5}B_{15}$ amorphous wire. This composition is called 'zero magnetostrictive' because its magnetostriction is very small. After thermal annealing, the magnetostriction becomes positive. The tensile stress derivative of magnetostriction, defined phenomenologically as $A = \mathrm{d}\lambda/\mathrm{d}\sigma$, is known [6, 7] to be negative in most experiments. This is true also for annealed wire. Therefore we expect that λ will change with torsional strain towards more negative values. Instead, we have found [5] a systematic reduction in the absolute value of λ with torsion. In particular, for an as-quenched sample we obtain an increase in λ (which is negative in this case). Also, the absolute value of the constant A is found [5] to be reduced with increasing torsion. The main idea of this paper is that this behaviour could be due to quenching of the Joule magnetostriction λ by torsional deformation of the crystal-field potential.

The magnetic anisotropy of crystals is usually calculated by integrating the contributions from particular electronic states over the Brillouin zone (BZ); there, a small part of the zone near the high-symmetry axis and the Fermi level is known to give the major contribution to the energy of magnetic anisotropy [8]. Then, the theoretical description of the effect can be limited to this small part of the BZ [9]. In amorphous materials, we have no BZ but we still have the density of electronic states. Some of these states certainly have a non-zero orbital

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magnetic moment, because amorphous materials are magnetostrictive as also are crystalline materials. The relation of these states to the amorphous structure remains unclear. Some explanation of this problem may be due to the long range of the ferromagnetic exchange interaction, which averages out local magnetic anisotropy within large clusters of atoms [10]. This problem is not within the scope of our paper, and our model description is to be taken as phenomenological. In principle, the model is the same as applied before [11] to the calculation of the constant A for a similar amorphous alloy composition.

The organization of the paper is as follows. First, we briefly report the data which are to be explained. In subsequent sections, our model calculations are described and the results are discussed in the context of experimental data. Final conclusions close the paper.

2. Experimental data

Amorphous $(Co_{95}Fe_5)_{72.5}Si_{12.5}B_{15}$ wire of diameter 0.12 mm was cut into pieces, of 10 cm length. The magnetostriction λ and its strain derivative A were measured [5] by means of the small-angle magnetization rotation method. In this method, the measured signal is known [12] to be proportional to the actual values of saturation magnetization M_s. For zero torsion, the value of λ was found to be about -4×10^{-8} for an as-quenched sample, and $+1 \times 10^{-7}$ for annealed wire. The results are given in figures 1 and 2. The observed asymmetry with respect to torsion should be assigned to a torsional stress, which is quenched in the amorphous structure [13]. This asymmetry vanished after annealing, as can be seen in figure 2. The observed values of the coefficient A were found [5] to be not influenced by annealing. At zero torsion, A was equal to -1.6×10^{-10} MPa^{-1} and varied smoothly to -1.0×10^{-10} MPa^{-1}, when the torsion ξ was 20π rad m^{-1}. As we can see in figures 1 and 2, the absolute value of magnetostriction λ is reduced with torsion both for as-quenched ($\lambda < 0$) and for annealed ($\lambda > 0$) wire.

This behaviour is unexpected for the following reason: almost everywhere in the volume of a wire, torsional stress can be seen as a tensile stress along an axis forming an angle $\pi/4$ with the axis of a wire [14]. As long as the amorphous structure can be seen as isotropic, its magnetoelastic behaviour is governed by the linear magnetoelastic constant λ. We have found that the tensile stress derivative of λ is negative; despite that, λ increases with increasing torsional stress for the as-quenched sample. So, there is a basic difference between the influence of tensile and torsional stresses on magnetostriction λ, and our intention is to determine this difference.

In principle, the magnetization dependence on torsion (the inverse Wiedemann effect (IWE)) could be responsible, at least partially, for the above difference. We have made an attempt to separate out this effect. This is done on the assumption that the observed [5] torsion dependence of the constant A, namely $A(\xi)$, can be assigned to the IWE. Then we can use this dependence to determine the curve $M_s(\xi)$ and to substitute it into the experimental data on $\lambda(\xi)$. In this way we get from the experimental data the 'renormalized' magnetostriction λ_{ren}, which depends on the torsion but not through the IWE. The results on λ_{ren} are given in figures 1 and 2. These results should be compared to the values of λ_{cal} given by the expression

$$\lambda_{cal}(\xi) = \lambda(0) + A\langle\sigma(\xi)\rangle \tag{1}$$

where $\langle\sigma(\xi)\rangle = \langle\xi r\rangle$ is the torsional strain averaged over the wire volume. For simplicity, we adopt $A = A(\xi = 0)$; this does not influence the conclusion that $\lambda_{ren}(\xi)$ cannot be fitted by $\lambda_{cal}(\xi)$ for as-quenched wire. Then, the observed torsional dependence of magnetostriction cannot be explained by means of the IWE, and another interpretation of

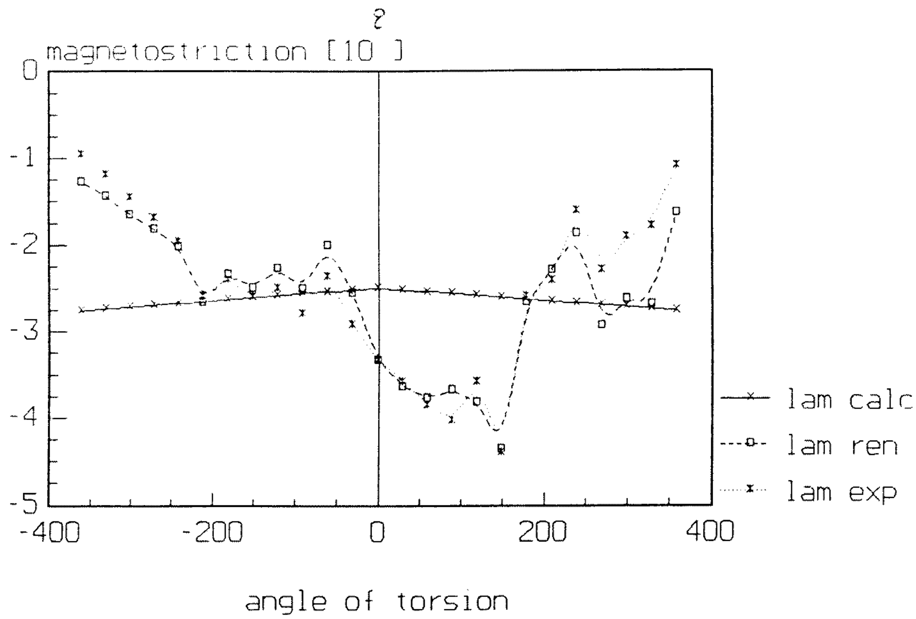

Figure 1. Experimental dependence of the magnetostriction λ for as-quenched (Co,Fe)–Si–B amorphous wire [5], the torsional dependences of renormalized magnetostriction and the curve λ_{cal} (equation (1)).

the experimental data is needed. In the next section we argue that the solution is provided by the idea of quenching the orbital magnetism by the torsional stress.

3. Model calculations

The starting point is the Stoner-like model band [11]. The Hamiltonian includes the spin–orbit interaction, the Zeeman spin, the orbital terms and the coupling of orbital energy to the crystal field:

$$H = G\boldsymbol{L}\cdot\boldsymbol{\sigma} - 2\mu_B\Delta\cdot(\boldsymbol{\sigma}+\alpha\boldsymbol{L}) + H_\varepsilon \tag{2}$$

where G is the one-electron spin–orbit constant, $\boldsymbol{L}$ and $\boldsymbol{\sigma}$ are orbital and spin operators, μ_B is the Bohr magneton and Δ is an effective magnetic field which is equivalent to the Stoner gap. The magnetoelastic Hamiltonian is diagonal in spin index; its matrix representation in the t_{2g} basis is

$$H_\varepsilon = \begin{bmatrix} -b\varepsilon & 0 & 0 \\ 0 & -b\varepsilon & br\xi \\ 0 & br\xi & 2b\varepsilon \end{bmatrix} \tag{3}$$

where b is a microscopic magnetoelastic coefficient. Here, both tensile ε and torsional ξ strains are taken into account. The t_{2g} basis is the minimal basis which captures the three-dimensional space; the e_g bands are omitted for simplicity. We would like to add that our model description is limited to a small fraction of electronic states, where the orbital moment is different from zero; this approach, although phenomenological, was found [9, 11] to be useful. The effective density of states is shown in figure 3. The calculations are limited to the case of a strong ferromagnet (large Stoner gap), i.e. we neglect the spin–orbit matrix

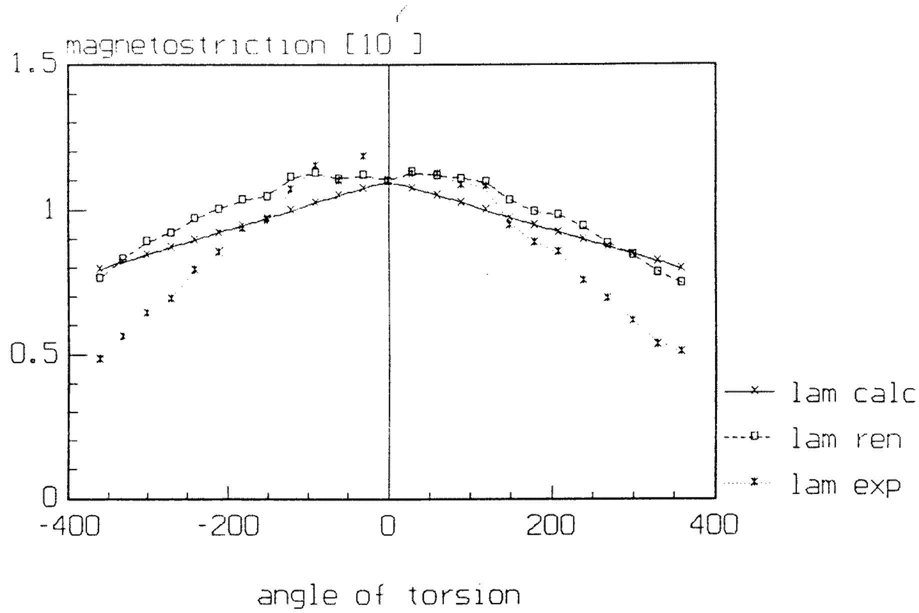

Figure 2. Experimental dependence of the magnetostriction λ for annealed (Co,Fe)–Si–B amorphous wire [5], the torsional dependences of renormalized magnetostriction and the curve λ_{cal} (equation (1)).

elements which are non-diagonal in spin variable. These matrix elements, if taken into account as a perturbation, produce corrections to the eigenvalues which are proportional to $1/\Delta$, where Δ is the Stoner gap. The torsion energy is taken into account as a perturbation within the second-order perturbation calculation. We get the eigenvalues

$$E_1 = -\Delta - b\varepsilon + |G/2 - \alpha\Delta| + \frac{(br\xi)^2}{|G - 2\alpha\Delta| - 6b\varepsilon} \tag{4}$$

$$E_2 = -\Delta - b\varepsilon - |G/2 - \alpha\Delta| + \frac{(br\xi)^2}{-|G - 2\alpha\Delta| - 6b\varepsilon} \tag{5}$$

$$E_3 = -\Delta + 2b\varepsilon + \frac{(br\xi)^2}{6b\varepsilon - |G - 2\alpha\Delta|} + \frac{(br\xi)^2}{6b\varepsilon + |G - 2\alpha\Delta|} \tag{6}$$

where $\alpha\Delta$ is the orbital polarization [15], ξ is the torsion and r is the distance between a given point of the wire and the wire axis. The remaining three energy levels can be obtained from the relation

$$E_i(\Delta) = E_{i-3}(-\Delta) \qquad i = 4, 5, 6. \tag{7}$$

The magnetic anisotropy energy U is written in the form

$$U = \sum_{i=1}^{6} \int_{-\infty}^{\mu} e\rho(e - E_i)\, \mathrm{d}e \tag{8}$$

where e is an energy variable, μ is the chemical potential and ρ is a model function of the density of electronic states:

$$\rho(e) = \sum_{i=1}^{6} \frac{d}{6\pi} \frac{1}{(e - E_i)^2 + d^2} \tag{9}$$

where d is the half-bandwidth.

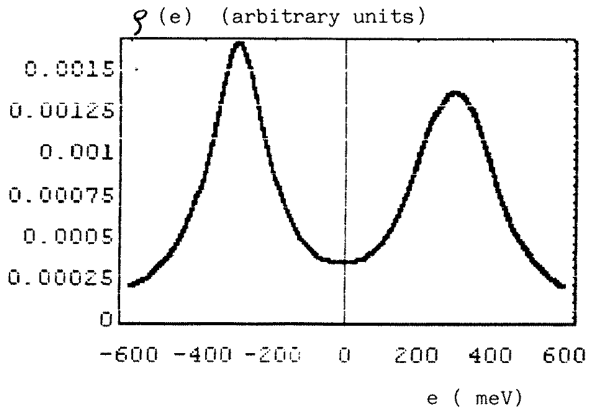

Figure 3. Density of states according to equation (9).

The magnetostriction λ is calculated within the rigid-band model [9] as

$$\lambda = -\frac{1}{c} \sum_{i=1}^{6} n_i \frac{\partial E_i}{\partial \varepsilon} \tag{10}$$

where n_i is the number of electrons in the ith state and c is an appropriate elastic constant. Let us disregard for a moment the torsion dependence of n_i, which is justified for wide bands, and let us consider the case of a strong ferromagnet with less than half the band filled, where $n_4 = n_5 = n_6 = 0$. The tension stress derivatives are performed at $\varepsilon = 0$. Then, for a given point r of a wire, we get

$$\lambda(r, \xi) = b(2n_3 - n_1 - n_2) \left\{ 1 - 6 \left[\frac{br\xi}{G - 2\alpha\Delta} \right]^2 \right\} = \lambda(\xi = 0) \left\{ 1 - 6 \left[\frac{br\xi}{G - 2\alpha\Delta} \right]^2 \right\} \tag{11}$$

where $\lambda(\xi = 0)$ does not depend on r. Averaging over the volume of a wire, we get

$$\lambda(\xi) = \lambda(0) \left\{ 1 - 3 \left[\frac{bR\xi}{G - 2\alpha\Delta} \right]^2 \right\} \tag{12}$$

where R is the wire radius. As we can see from equation (12), the absolute value of λ is reduced by the torsion ξ, exactly as in the experiments, for both the as-quenched sample and the annealed sample.

This result motivates us to perform numerical calculations for six subbands, where the torsion dependence of the numbers of electrons is taken into account. The values of the parameters and the model density of states for this calculation are taken from [11], except for the Stoner gap and the band filling. These values are given in table 1. We would like to note, however, that the model band structure is not exactly the same as in [11] even for zero torsion, because our present assumption on strong ferromagnetism has not been made in that work. This approximation is too rough to calculate the stress derivative A of magnetostriction, because the expression for A [11] contains the second derivative of energy levels with respect to the strain;

$$-c^2 A = \sum_i n_i \frac{\partial^2 E_i}{\partial \varepsilon^2} - \rho_i(\mu)\left(\frac{\partial E_i}{\partial \varepsilon}\right)^2 + \left(\sum_j \rho_j(\mu)\frac{\partial E_j}{\partial \varepsilon}\right)^2 \Big/ \sum_k \rho_k(\mu) \tag{13}$$

and here this second derivative is zero for zero torsion (equations (4)–(6)). For wide bands, ρ is small and other contributions to A in equation (13) are negligible. Still we believe that the torsion dependence of magnetostriction can be discussed even within the above simplified picture. Band calculations are performed with the condition that the Stoner gap is not changed with torsion. The results are given in figure 4 and compared to the renormalized values of magnetostriction λ. In this way we exclude the torsion dependence of magnetization also from experimental data.

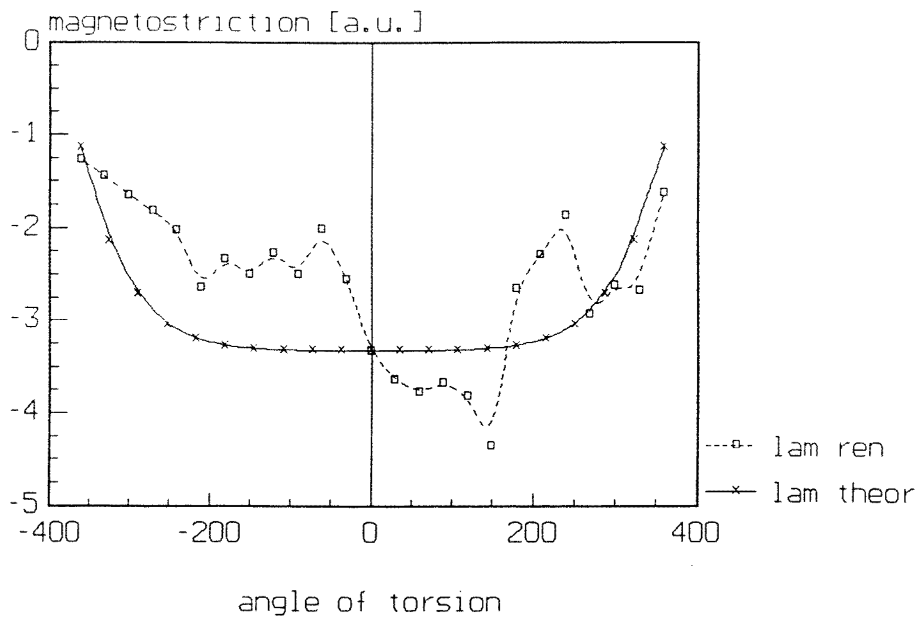

Figure 4. Renormalized magnetostriction for the as-quenched amorphous state compared with the results of model band calculations (a.u., arbitrary units).

4. Discussion

The analytical solution for $\lambda(\xi)$ given by equation (12) is a purely parabolic curve, which always leads to a reduction in the absolute value of the magnetostriction with increasing torsion. This shape is only slightly changed in the numerical solution (figure 4), where the torsion dependence is less smooth than a parabola. In both cases, we have to admit that the torsional strain energy is comparable to the difference between the energies of electronic states for the same orientation of spin. If the torsional strain energy is too large on this scale, our perturbational approach is not valid. If it is too small, we get the model prediction that magnetostriction does not depend on torsion. This seems to be the case for the annealed sample (figure 2). This lack of dependence could be obtained very easily for the values of the Stoner gap different from that in table 1. That is why we do not perform any comparison to experimental data for the case of the annealed wire (figure 2).

Table 1. Values of parameters for numerical fitting the experimental data on the torsional dependence of magnetostriction in $(Co_{95}Fe_5)_{72.5}Si_{12.5}B_{15}$ amorphous wire.

Spin–orbit coupling G (meV/atom)	30
Half-bandwidth of Lorentzian density of states (meV/atom)	100
Microscopic magnetoelastic constant b (meV/atom)	74
Stoner gap Δ (meV/atom)	299.5
Band filling (electrons/atom)	0.2
Orbital polarization coefficient α (dimensionless)	0.05

The direct result of both analytical and numerical calculations is that the variation in λ with torsion is visible only within a small range of magnetizations, but the evaluation of this range is rather difficult. With the value of the microscopic magnetoelastic parameter $b = 0.074$ eV, we find the energy of torsion comparable to 10^{-4} eV. The above-mentioned difference between the energy levels is due to the spin–orbit interaction energy and to the orbital polarization [15]. For the former, we have no direct evaluation. Reference data give us a value between 0.01 and 0.1 eV [16]. The latter is dependent on the magnetization and, thus, on the temperature. Moreover, the temperature dependence of the magnetization is known to be hardly understood within the Stoner model. In fact, we expect that, in 3d metals, local magnetic moments are not much influenced by temperature, and they are different from zero above the Curie temperature [16]. Therefore, the small value of the energy gap between orbital states could be more stable with temperature than it appears from the Stoner model. These arguments allow us to treat our calculation as a qualitative estimation of the investigated effect. On the other hand, the quenching of orbital magnetism can be only one of several effects contributing to the data observed experimentally [5]. Another mechanism could be analogous to those which were referred to when discussing the tensional stress dependence of the magnetostriction: variations in the distribution of pairs of atoms [17], fluctuations in local magnetostriction [18] or stress dependence of anisotropies of local clusters [19]. This work is a continuation of our previous attempts [4, 9, 11] to deduce the macroscopic magnetoelastic behaviour of metallic magnets directly from microscopic band effects. Until now, we have no direct experimental criterion to separate the contributions to magnetostriction produced by various mechanisms. That is why we believe that band effects should be kept in the list of possible contributors to the energy of magnetoelastic coupling in amorphous magnets.

It is not clear whether the effect of quenching of magnetostriction can be observed for other compositions, where the value of magnetostriction is far from zero (e.g. Co–Si–B and Fe–Si–B). The tensile stress dependence of magnetostriction was not observed here, and it seems that the effect is too small to be detected if the magnetostriction is of the order of 10^{-6} or more. However, the matrix elements of the tensile stress energy operator are different from those of the torsional stress energy, and the value of λ can, in principle, be changed even with a relatively small energy of torsion. Such a dependence would be of great importance for numerous applications. In the case of wires, we could obtain a radial distribution of magnetostriction just by the application of torsional stress.

5. Conclusions

The effect of torsional strain on magnetostriction in amorphous zero-magnetostrictive wire is investigated within a simple Stoner-like band model. We find that the thermal average of the magnetoelastic coupling energy is reduced by the matrix elements of the torsional energy operator, which are non-diagonal in the base of eigenstates of the orbital magnetic moment. Both analytical and numerical calculations are presented; for the latter, a set of parameters is found where the results agree with recently observed data on as-quenched Co–Fe–Si–B amorphous wire.

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