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Torque relaxation in Dzyaloshinskii–Moriya spin glasses: a numerical study

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Abstract. We present results obtained from a Monte Carlo simulation of the torque relaxation in a classical Ruderman–Kittel–Kasuya–Yosida spin glass in the presence of weak anisotropic Dzyaloshinskii–Moriya interactions. The simulations are carried out at zero temperature and correspond to the short-time results observed in experiments. For weak anisotropy, the results are consistent with those seen in experiments on **Cu**Mn in the short-time limit. For strong anisotropy the qualitative features seen in the simulation are interesting and should be checked in experiments.

1. Introduction

The microscopic origin of the anisotropy in transition-metal spin-glass alloys (such as **Cu**Mn or **Ag**Mn), observed in a variety of experiments (for a recent review, see [1]), has been traced [2] to a Dzyaloshinskii–Moriya (DM) interaction arising from spin–orbit scattering of the conduction electrons. This mechanism explained the dramatic enhancement of the anisotropy energy produced by the addition of non-magnetic impurities with strong spin–orbit coupling (such as Pt or Au). Subsequently, several researchers [3–5] argued from general symmetry considerations that, when a weak DM interaction is present, the increase in energy due to rotation of the spin system from a frozen metastable state is given by

$$\Delta E = K(1 - \cos\theta) \tag{1}$$

where θ is the rotation angle and the anisotropy constant K is independent of the rotation axis. The macroscopic anisotropy is thus unidirectional in the sense that ΔE is a 2π-periodic function of θ. In experiments on **Cu**Mn samples the anisotropy appears to be purely unidirectional [6] at least for rigid rotations at relatively small angles. Numerical simulation studies [7, 8] on **Cu**Mn spin glasses in the presence of weak DM anisotropy have also been successful in reproducing several qualitative features observed in electron spin resonance, hysteresis and torque experiments.

The dynamics of the anisotropy energy in **Cu**Mn spin glasses have also been studied in hysteresis [9] and torque [10] experiments. Following the notion of the macroscopic anisotropy as a remanent effect [11], some ideas were developed in [9] on the freezing of the anisotropy and hysteresis cycle experiments were present in support of these ideas. It was concluded that the remanent magnetisation and the anisotropy of spin glasses are

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two similar but independent (at least when the remanent magnetisation does not exceed a small fraction of the saturated magnetisation) properties associated with two different types of correlations—the remanent magnetisation represents correlations between the spins and the direction of the externally applied magnetic field and the anistropy represents correlations between the spins and the directions of local random anisotropy fields. On the contrary, in the torque relaxation study in [10], it was suggested that the decay of the anisotropy torque was governed by a different mechanism from that of the decay of remanent magnetisation. In a very recent experiment [12], extensive torque decay measurements were used to study the relaxation processes associated with remanent magnetisation and anisotropy in **Cu**Mn spin-glass alloys. From a comparison of relaxation of the anisotropy resulting from small-angle magnetic field rotations with relaxation of the remanent magnetisation, it was suggested that these two relaxations are controlled by the same mechanism, namely through local reorganisations of groups of spins. In a mean-field calculation of the consequences of rotational symmetry breaking in Heisenberg spin glasses in the presence of anisotropy, it was also suggested [13] that the macroscopic anisotropy decays to zero on the same time scale as the remanent magnetisation does. However, all the experiments described above are carried out on **Cu**Mn samples in which the strength of the anisotropy is relatively weak, and no systematic study is available in samples with various strength of anisotropic interactions (this could be done, for example, by adding different amounts of Pt or Au impurities to **Cu**Mn).

In this paper, we report results obtained from a Monte Carlo simulation of the torque relaxation in a classical Ruderman–Kittel–Kasuya–Yosida (RKKY) spin-glass model in the presence of weak DM anisotropy of various strengths. Since the present study is carried out at zero temperature and the physical time associated with a Monte Carlo simulation of several thousand of steps per spin is very short compared with experimental time scales of torque relaxations, detailed comparison with experiments is difficult. However, for weak anisotropy the simulation results compare favorably with the available experimental data over 'short' times for **Cu**Mn. On the contrary, very few experimental data on torque relaxation for strong anisotropy systems exist in the literature and the qualitative features seen in the simulation in this case should be checked on laboratory samples.

The rest of the paper is organised as follows: § 2 contains a definition of the model studied in this paper and a brief description of the numerical procedure employed. in § 3, we present the results of the numerical experiments, and § 4 contains a brief discussion and conclusions.

2. Model and numerical procedure

The system studied here corresponds to $CuMn_xT_y$, where T represents a non-magnetic impurity that mediates the DM interaction and x and y denote concentrations. The model consists of a system of classical Heisenberg spins interacting via isotropic RKKY and weak DM interactions. We consider a $L \times L \times L$ FCC lattice with periodic boundary conditions. Spins are placed at $N = 4xL^3$ randomnly chosen sites and spin–orbit scatterers are placed at $N_i = 4yL^3$ other sites, also chosen at random. The Hamiltonian of the system in the presence of a uniform magnetic field $\boldsymbol{h}$ is given by

$$H = H_{\mathrm{RKKY}} + H_{\mathrm{DM}} - \sum_i \boldsymbol{h} \cdot \boldsymbol{S}_i. \tag{2}$$

For the RKKY term, we used

$$H_{\mathrm{RKKY}} = -J_0 \sum_{j>i} \frac{\cos(2k_{\mathrm{F}} r_{ij})}{r_{ij}^3} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{3}$$

where $\boldsymbol{S}_i$ is the spin of unit length at site i and r_{ij} is the distance between sites i and j. For the lattice constant and the Fermi wavevector k_{F}, values appropriate for Cu were used. Following [14] a system of reduced units (ru) in which J_0/r_{ij}^3 is set equal to unity for ij nearest neighbours, is used. For the DM interaction

$$H_{\mathrm{DM}} = -V \sum_{i>j} \sum_k \left[\sin\left(k_{\mathrm{F}}(r_{ij} + r_{jk} + r_{ik}) + \frac{\pi}{10} Z_{\mathrm{d}} \right) \right] \times \frac{(\boldsymbol{r}_{ik} \cdot \boldsymbol{r}_{jk})[(\boldsymbol{r}_{ik} \times \boldsymbol{r}_{jk}) \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_j)}{r_{ik}^3 r_{jk}^3 r_{ij}}. \tag{4}$$

In equation (4), Σ_k represents a sum over all sites occupied by the spin–orbit scattering impurity T and Z_{d} is the number of d electrons in T. We took $V/J_0 = 0.2$ and $Z_{\mathrm{d}} = 9.4$ which are appropriate for T ≡ Pt. To avoid multiple interactions arising from periodic boundary conditions, the interaction was set equal to zero if any one of the distances r_{ij}, r_{ik} and r_{jk} was larger than $L/2$.

The numerical study consisted of locating metastable equilibrium configurations (EC) of spin system in both the presence and the absence of external magnetic field. The EC were generated by using the algorithm in [14]. In this procedure the spins are updated one at a time. In the update of spin $\boldsymbol{S}_i$, one first calculates the instantaneous local field $\boldsymbol{H}_i$ and then sets $\boldsymbol{S}_i$ parallel to $\boldsymbol{H}_i$. An iteration step (or equivalently a Monte Carlo step at zero temperature) is defined as a block of N consecutive updates. In this process, the system is not allowed to go over any energy barrier during its relaxation. Convergence to an EC was determined from the rate of change in the total energy. Since the energy decreases very slowly as the system closely approaches an EC, we calculated the energy after every 50 iterations for better accuracy. The iteration was stopped when the fractional change in energy in the last 50 iterations was less than 10^{-8}.

3. Results of numerical experiments

The results reported in this section were obtained from simulations of three groups of 10 samples, each containing 161 spins distributed in a 20^3 lattice with concentration $x =$ 0.5 at.%. The typical error bars associated with the quantities measured are about 5%. In the first group the number N_i of spin–orbit scatterers was 8 ($y = 0.025$ at.%), and the second and third groups contained 16 ($y = 0.05$ at.%) and 32 ($y = 0.10$ at.%) spin–orbit scatterers, respectively. In the torque relaxation experiment, we used three different protocols closely following real experiments [12].

(i) In the FCθ protocol, the sample is subjected to field cooling (FC) under a field h set along the Z axis, i.e. the sample is relaxed in a field h until it reaches sufficiently close to an EC. The field is then rotated through an angle $\theta = 5°$ about the X axis at $t = 0$. The system is relaxed towards a new EC by the algorithm discussed in § 2 and the torque is

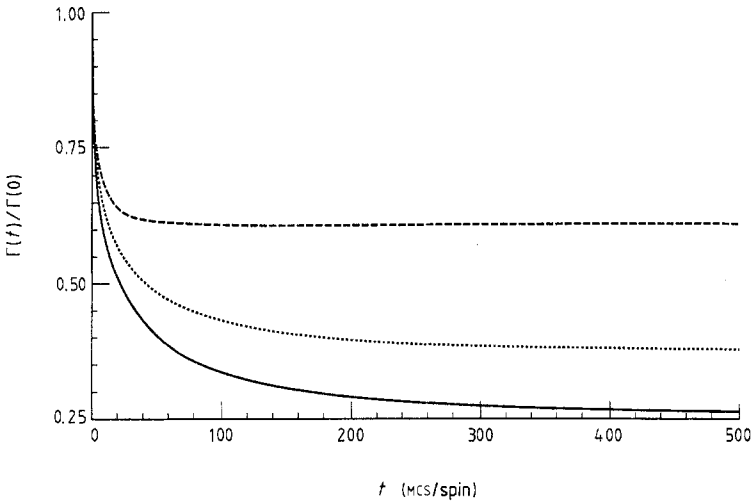

Figure 1. Normalised torque against time measured in units of Monte Carlo steps per spin (MCS/spin) in the FCθ protocol for different concentrations y of spin–orbit scattering impurity ($H = 9$ kG; $\theta = 5°$): - - -, $y = 0.1$ at.%; · · · ·, $y = 0.05$ at.%; ——, $y = 0.025$ at.%.

calculated at every step of iteration as $\Gamma = |\boldsymbol{M} \times \boldsymbol{h}|$ where $\boldsymbol{M}$ is the total magnetisation given by $(1/N)\Sigma_i \boldsymbol{S}_i$.

(ii) In the FCσ protocol, after FC in h, the field is set at a low value h' along the Y axis. The system is then relaxed to a new EC and the torque is calculated at every step of the evolution.

(iii) In the ZFCθ protocol, after zero-field cooling (ZFC), a large field h is set along the Z axis and a new EC is located. Then the field is rotated by an angle $\theta = 5°$ about the X axis at $t = 0$. The system is then relaxed to a new EC and the torque is calculated at every step of the iteration.

Assuming that the anisotropy energy has only a unidirectional form and a rigid spin structure, the torque Γ for an applied field at an angle η to the anisotropy axis is given by [12]

$$1/\Gamma^2 = \frac{1}{(\sigma h)^2} + [(K \cos \eta + \sigma h)/\sigma h K \sin \eta\,]^2 \tag{5}$$

where σ is the effective irreversible magnetisation. In the torque relaxation study, one is particularly interested in two simplifying limits: one when the applied magnetic field is much stronger than the anisotropy and the other when the external field is weak compared with the strength of the anisotropy. In simulation of $\mathbf{CuMn}_x\mathbf{Py}_y$ spin glasses [8] it was estimated that $K = 4.5 \times 10^{-4}$ ru ($\simeq 1.5$ kG) for $x = 0.5$ at.% and $y = 0.1$ at.%. Hence we kept $h = 9$ kG to be in the strong-field limit and $h' = 50$ G to be in the weak-field limit, similar to the field values in a recent experiment [12].

The results of the torque relaxation experiment in the protocol FCθ are shown in figure 1 for various concentrations of spin–orbit scatterers. In this figure the normalised torque $\Gamma(t)/\Gamma(0)$ is plotted against Monte Carlo steps. In these cases, we are in the strong-field limit ($h\sigma \gg K$) and $\Gamma = K \sin \eta$ from equation (5). One then expects to observe the relaxation of the anisotropy term $k \sin \eta$ in a strong applied field for various strengths of the anisotropy constant K. It can be seen from figure 1 that for any value of

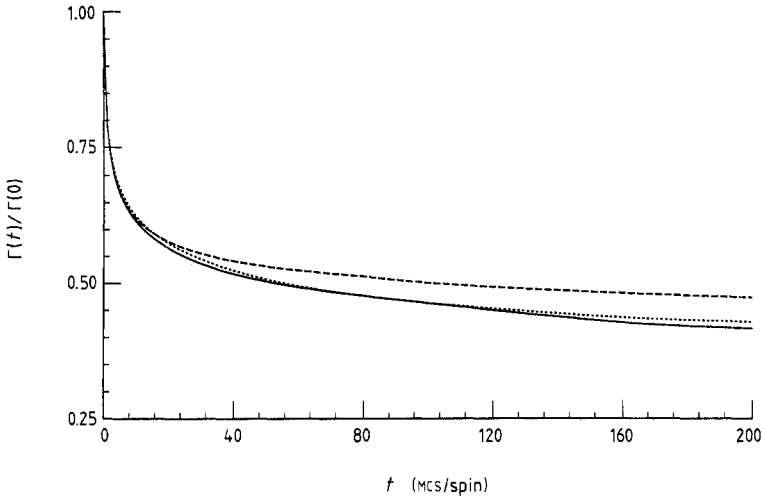

Figure 2. Normalised torque against time measured in units of Monte Carlo steps per spin (MCS/spin) in the FCθ protocol for different concentrations y of spin–orbit scattering impurity (H = 50 G): - - -, y = 0.1 at.%; · · · ·, 0.05 at.%; ——, 0.025 at.%.

the anisotropy the torque does not decay to zero within available computer time. We note that, as the concentration of Pt impurities is increased, the torque freezes to a relatively larger value. This is consistent with the fact that the anisotropy constant K increases as the concentration of spin–orbit scatterers are increased [2]. It also suggests that for stronger anisotropies the freezing of correlations between the spins and the local anisotropy fields is stronger.

In figure 2, we present the torque relaxation data for one of the other protocols, FCσ. The situation is quite different in this case and the torque relaxation in this protocol depends very weakly on the strength of the anisotropy, as expected from the weak-field limit, $h\sigma \ll K$ of equation (5), i.e. $\Gamma \simeq \sigma h \sin \eta$. It is also found that the torque signal in the FCσ protocol is proportional to the remanent magnetisation m_r even for strong anisotropy, as shown in figure 3.

We now turn to the ZFCθ protocol. The results for different strengths of anisotropy are shown in figure 4 (curves B_1, B_2 and B_3), along with the FCθ curves (curves A_1, A_2 and A_3). For weak anisotropy, we find that these two curves are almost identical as shown in figure 4 (curves B_1 and A_1). In the weak-anisotropy case, the effects of the magnetic field dominates and the EC to which the system relaxes when the field is turned on after ZFC is perhaps the same one as that obtained in FC. If this is true, then the asymptotic values of the torques should be the same in both cases. This is what we see in the simulation and, apparently, this is also observed in experiments on **CuMn**—the short-time values of the torque are the same in FCθ and ZFCθ protocols in figure 2 of [12]. We note that, if the anisotropy is strong, then the initial EC obtained after ZFC has spin orientations favourable to the anisotropy energy. When the field is turned on, the spins adjust locally to the field. The resulting EC may not be optimal for the anisotropy energy. This might explain why the torque observed in ZFCθ is less than that for FCθ for strong anisotropy, as shown in figure 4 by curve A_2–B_2 and curve A_3—B_3. It would be interesting to determine experimentally whether the short-time values of the torque are different in FCθ and ZFCθ if the anisotropy is strong.

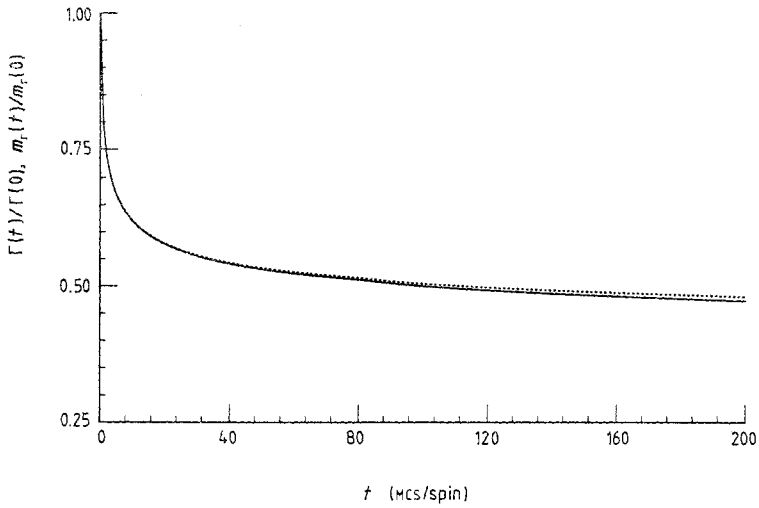

Figure 3. Normalised torque $\Gamma(t)/\Gamma(0)$ (——) and normalised remanent magnetisation $m_r(t)/m_r(0)$ (· · ·) against time measured in units of Monte Carlo steps per spin (MCS/spin) in the FCσ protocol. The concentration y of the spin–orbit scattering impurity Pt is 0.1 at.%; the concentration x of Mn is 0.5 at.%; the applied field is 50 G.

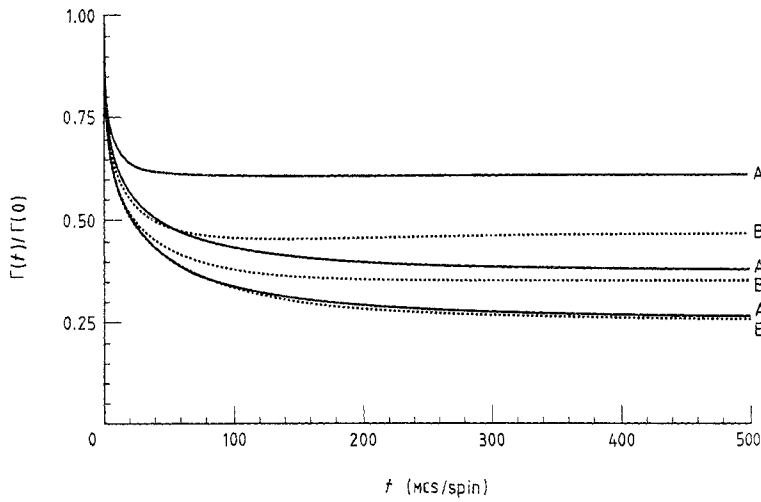

Figure 4. Normalised torque against time measured in units of Monte Carlo steps per spin (MCS/spin) in the FCθ (curves A_1, A_2 and A_3) and ZFCθ (curves B_1, B_2 and B_3) protocols. The concentrations of spin–orbit scattering impurity are as follows: curves A_1 and B_1, 0.025 at.%; curves A_2 and B_2, 0.05 at.%; curves A_3 abd B_3, 0.1 at.%. The applied field is 9 kG.

4. Conclusions

We note that the torque relaxations seen in this zero-temperature simulation are simply for the approach to the nearest EC (in a zero-temperature simulation the possibility of transitions over barriers are not built in), whereras the torque relaxation observed in

experiments involves transitions among ECs. Also, the physical time associated with a Monte Carlo simulation of several thousand steps per spin is about 10^{-8} s, whereas in experiments the torque relaxes over time scales of minutes or even hours. In this situation the asymptotic value of the torque obtained in the simulation should correspond to the 'short-time' value observed in experiments. We believe that a proper simulation of the process of torque relaxation observed in experiments would have to be done at a non-zero temperature, taking into account the correct dynamics of the Heisenberg spins. This, of course, would be a much more difficult calculation. The results of this simulation are, nevertheless, consistent with experiments in the 'short-time' limit for weak anisotropy. For strong anisotropy the qualitative features seen in the simulation should be checked in experiments on ternary spin glasses.

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