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Monte Carlo Simulation of Random-Anisotropy Amorphous Magnets

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Abstract. Using the Monte Carlo method, within the frame of the Heisenberg model, we studied the magnetic properties of amorphous Tb. The relaxation of magnetization of the model of amorphous Tb was studied. We established that the relaxation goes in two stages. On the first stage the magnetization sharply decreases by some amount $\Delta M_z$, on the second stage the magnetization decreases with time according to the logarithmic law. The possible mechanisms of relaxation is discussed.

1. Introduction
Amorphous alloys based on rare-earth metals are of great interest due to their unique magnetic properties [1-3]. Particularly, the Re-Tb amorphous alloys transit into the spin-glass-like state at low temperatures. The nature of the spin-glass state in amorphous alloys is yet poorly understood. This encourages us to construct and analyze computer models of these materials. In this paper we report on the Monte Carlo simulation of magnetization relaxation in pure amorphous terbium. Its properties have to be close to that of amorphous alloys with high concentrations of the terbium atoms.

2. Simulation technique
Using the molecular dynamics method, at $T = 100$ K we constructed the models of atomic structure of pure amorphous terbium containing 100 000 atoms in a cubic cell with periodic boundary conditions. The interatomic interaction was described by an empirical polynomial potential [4]. The parameters of the potential were estimated by the values of bulk modulus, atomization energy, atomic volume, and the interatomic distance for crystalline Tb. Application of this potential for the models of Re-Tb amorphous alloys revealed a good agreement of the model and experimental radial distribution functions and parameters of the topological short-range order [5].

Magnetic properties of these models were studied using the Monte Carlo method within the standard Metropolis algorithm [6, 7], in the framework of the Heisenberg model. For the model of amorphous Tb we used the Hamiltonian proposed by Harris, Plischke and Zuckermann for amorphous alloys containing rare-earth atoms with the non-zero orbital moment [8]:

$$H = -\frac{1}{2} \sum_{i,j} J_{ij}(S_i \cdot S_j) - D \sum_i (n_i \cdot S_i)^2 - \mu H \sum_i S_i^z,$$

(1)

where $J_{ij}$ is the integral of the exchange interaction between atoms $i$ and $j$; $D$ is random anisotropy; $S_i$ is Heisenberg spin; $n_i$ is unit vector determining the directions of the local anisotropy axes, which were chosen
randomly in each site: \( \mu = 9.72 \mu_0 \) is effective magnetic moment of the Tb atom; \( h \) is external magnetic field strength.

Magnetic moments of the Tb atoms interact by means of the long-range RKKY exchange mechanism [9]. The exchange interaction integral rapidly decreases with the interatomic distance, therefore the positive (ferromagnetic) interaction between the nearest neighbours brings the maximal contribution to the exchange energy.

As an approximation of the RKKY interaction between the moments of the Tb atoms, we chose the linear dependence of the exchange integral on the interatomic distance \( r \) [10]:

\[
J(r) = \begin{cases} 
J_0 \frac{r_{\text{min}} - r}{r_{\text{min}} - r_1}, & r \leq r_{\text{min}} \\
0, & r > r_{\text{min}} 
\end{cases}
\]

(2)

where \( J_0 = 19.26 \) K is the average value of the exchange integral fitted such that the temperatures of the magnetic phase transitions \( T_j \) would be close to the experimental values of \( T_j \) for the Re-Tb amorphous alloys; \( r_1 \) is the first peak position on the partial pair radial distribution function \( g_{\text{Tb-Tb}}(r) \); \( r_{\text{min}} = 0.446 \) nm is the position of the first minimum of the \( g_{\text{Tb-Tb}}(r) \) function. As the distribution of the interatomic distances in the first coordination sphere of an amorphous metal is close to normal law so the distribution of the exchange integrals \( J_0(r) \) is also close to normal law.

The value of the anisotropy \( D \) in this paper varied in a wide range (\( D/J_0 = 0 \rightarrow 20 \)).

It is known from literature that for the crystalline terbiurn the anisotropy constant is \( 5.5 \times 10^8 \) erg/cm\(^3\) [9], or \( 127 \) K/at. When a material transforms from the crystalline state into the amorphous one the value of the anisotropy constant practically does not change [11]. So the basic value of the anisotropy constant for amorphous Tb was chosen as \( D = 127 \) K, or \( D/J_0 = 127/19.26 \approx 6.6 \).

Cooling of the models was conducted from the paramagnetic state in the temperature interval \( T = 100 \rightarrow 1 \) K with steps \( \Delta T = 2, 5 \) and \( 10 \) K. During cooling, we calculated the temperature dependencies of the potential energy (1) and magnetization by the formula:

\[
\bar{M} = \frac{1}{N} \sum_i \sqrt{(S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2},
\]

(3)

where \( N \) is number of spins in the system, \( \langle \ldots \rangle \) is time averaging during \( 10^3 \) MC-steps/spin.

Magnetic susceptibility \( \chi \) was calculated by numerical differentiation of magnetization by external magnetic field strength:

\[
\chi = \frac{\Delta M}{\Delta H}.
\]

(4)

It was established that in the studied models in the fields of \( 0 \rightarrow 5 \) kOe the magnetization depends on the field linearly. This allows us use the eq. (4) with the good accuracy and to assume \( \Delta H = 5 \) kOe.

3. Results and discussion

We studied the relaxation of the magnetization in the model of amorphous Tb at various values of the anisotropy (\( D/J_0 = 0, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20 \)). For every value of \( D/J_0 \) the calculation was carried out at the constant temperature \( T = 1 \) K. The external magnetic field with the strength 1000 kOe along the \( Oz \) axis was switched on immediately, then the system was maintained in the field during \( 9 \rightarrow 20 \) cycles of \( 10^3 \) MC-steps/spin until the magnetization achieved saturation (from 0.999 at \( D/J_0 = 0 \) to 0.93 at \( D/J_0 = 20 \)). Then the field was switched off and the time dependence of the projection of the magnetization on the \( z \) axis \( \bar{M}(t) \) was studied.

At all studied values of \( D/J_0 > 0 \) the magnetization relaxation goes in two stages. On the first stage that proceeds immediately after the switching off the magnetic field, the magnetization sharply (during 1–2 cycles of \( 10^3 \) MC-steps/spin) decreases by some amount \( \Delta M_1 \). With increasing the \( D/J_0 \) ratio the value of the magnetization jump monotonically increases (Fig. 1) and probably comes to a constant value ~0.4 at
On this stage we observe the disorientation of magnetic moments of the Tb atoms from the state in which the spins are oriented in the direction of the external field to the state in which the orientation of the spins is determined mainly by the directions of the local anisotropy axes.

Fig. 1. Magnetization jump after switching off the external magnetic field for the model of amorphous Tb at $T=1$ K

On the second stage of the relaxation, the magnetization very slowly decreases with time without any signs of achievement of an equilibrium value. On this stage the magnetic moments of the Tb atoms turn by the small angles, which is due to competition between exchange interaction and random anisotropy.

To verify this assumption, we calculated the distribution functions $F(\theta)$ of angles between directions of the magnetic moments of the Tb atoms and directions of the corresponding random anisotropy axes at $D/J_0=6.6$ and $T=1$ K in the process of the magnetization relaxation (Fig. 2).

Fig. 2. Distribution function of the angles between directions of the spins and directions of the random anisotropy axes for the model of amorphous Tb at $D/J_0=6.6$ and $T=1$ K
In the moment directly before the switching off the external magnetic field, the $F(\theta)$ function has the almost uniform distribution over the angles from $-30^\circ$ to $-150^\circ$, since in the very strong fields ($H = 1000$ kOe) the magnetization is totally determined by the magnitude of the external field and the influence of the random anisotropy is negligibly small. In one cycle of $10^3$ MC steps/spin, after the switching off the external field, the $F(\theta)$ function undergoes the essential changes: two high maxima at $\theta = 20^\circ$ and $\theta = 160^\circ$ and a broad minimum at $\theta = 70^\circ - 110^\circ$ appear on it. This confirms the assumption of that at the first stage of the relaxation the spin reorientation takes place from the directions determined by the external field towards the directions close to those of the random anisotropy axes. Further the form of the $F(\theta)$ curve almost does not change, only the maxima become a little higher. In Fig. 2 the curve $F(\theta)$ calculated after 18 cycles of $10^3$ MC-steps/spin after switching off the external field is also given. Therefore, on the second stage of the relaxation the spin rotations by small angles take place that is caused by competition of the exchange interaction and random anisotropy.

In Fig.3 we present the time dependencies of a projection of magnetization on the $Oz$ axis for the model of amorphous Tb at various values of the $D/J_0$ ratio. It is seen that at $D/J_0=0$ magnetization with time remains practically constant. At the other values of $D/J_0$, the dependencies $M(t)$ decrease monotonically.

Fig. 3. Time dependence of the magnetization after switching off the external magnetic field for the model of amorphous Tb at $T = 1$ K

At all the values of the anisotropy constant, the dependence $M(t)$ was approximated by the least-square technique with a logarithmic function:

$$M(t) = a - b \cdot \ln t,$$

where $a$ and $b$ are fitting parameters.

It was confirmed experimentally that such a logarithmic relaxation of magnetization takes place in the real spin glasses [12-14]. With applying magnetic field to a sample, cooled to $T < T_f$ in zero field, magnetization first increases with a jump (in microscopic time), and then it slowly grows approaching to an equilibrium value according to the law close to logarithmic. If the sample is cooled in the field to $T < T_f$ then after the switching off the field the magnetization drops with a jump and then slowly decreases remaining finite even in time $10^5$ sec [14]. This feature proves that in spin glasses there is a wide spectrum of relaxation times that reaches the macroscopic times. The energy minima corresponding to the different sets of spin orientations are separated one from another by macroscopically high barriers, and thus the relaxation takes place in macroscopically large times.
For the model of amorphous Tb the magnetization relaxation was studied at $D/J_s = 6.6$ and various temperatures. In Fig. 4 we present the time dependencies of the projections of magnetization on the $Oz$ axis after switching off the external magnetic field calculated at the temperatures $10 – 70$ K with the step $10$ K. At the temperatures $T = 10 – 50$ K corresponding to the spin-glass state, the magnetization decreases with time very slowly, according to the logarithmic law (6). At the temperature $T = 60$ K close to the temperature of the spin-glass transition $T_f$, the magnetization decreases rapidly and fluctuate around zero. At the temperatures $T > 60$ K corresponding to the paramagnetic phase, the magnetization drops to zero very rapidly.

![Fig. 4. Time dependence of the magnetization after switching off the external magnetic field for the model of amorphous Tb at $D/J_s = 6.6$ and different temperatures](image)

4. References
[1] Fernandez-Baca J A and Wai-Yim Ching (ed.) 1995 *The Magnetism of Anorphous Metals and Alloys* (Singapore: World Scientific)
[2] Fukamichi K, Hattori Y and Goto T 1996 *Sci. Rep. RITU. Ser. A* 42 65
[3] Boucher B and Chieux P 1991 *J. Phys.: Condens. Matter* 3 2207
[4] Bataronov I L, Bondarev A V and Barmin Yu V 2000 *Bull. Russ. Acad. Sci. Phys.* 64 1329
[5] Bataronov I L, Bondarev A V, Urazov D V and Barmin Yu V 2005 *Bull. Russ. Acad. Sci. Phys.* 69 1299
[6] Binder K 1997 *Rep. Prog. Phys.* 60 487
[7] Binder K and Heermann D 1988 *Monte Carlo Simulation in Statistical Physics* (Berlin: Springer-Verlag)
[8] Harris R, Plischke M and Zuckermann M J 1973 *Phys. Rev. Lett.* 31 160
[9] Taylor K N R and Darby M I 1972 *Physics of Rare-Earth Solids* (London: Chapman and Hall)
[10] Bondarev A V 2008 *Bull. Russ. Acad. Sci. Phys.* 72 1251
[11] Chudnovsky E M 1988 *J. Appl. Phys.* 64 5770
[12] Lundgren L, Nordblad P and Svendlindh P 1986 *Phys. Rev. B* 34 8164
[13] Takayama H 2004 *J. Magn. Magn. Mater.* 272-276 256
[14] Dotsenko V S 1993 *Phys.-Usp.* 36 455