Monte Carlo simulation of amorphous magnets with random exchange interactions

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Abstract. Using the Monte Carlo method, the computer simulation of magnetic properties of pure amorphous Gd and Re-Gd amorphous alloys was performed. For the model of amorphous Gd the temperature dependencies of magnetization and magnetic susceptibility were calculated at different values of the ratio of exchange interaction integrals within the first and the second coordination spheres \(J_1 / |J_2|\). The magnetic phase diagram in coordinates \(T - J_1 / |J_2|\) was constructed. For the models of Re-Gd amorphous alloys the dependence of spin-glass transition temperature on concentration of Gd atoms was calculated. For all our models the hysteresis loops were calculated at different temperatures.

1. Introduction
Binary amorphous alloys of heavy rare-earth metals with nonmagnetic transition metals are of great interest due to their unique magnetic properties [1, 2]. In these systems the transition into the spin-glass state takes place. In amorphous alloys of the rhenium-gadolinium (Re-Gd) system the typical for spin glasses maximum on the temperature dependence of magnetic susceptibility \(\chi(T)\) and irreversibility of magnetization \(M(T)\) were experimentally revealed [3]. The spin-glass state occurs due to random exchange interactions in this system.

The nature of the spin-glass state on the microscopic level is studied insufficiently. In this connection, the computer simulation of atomic structure and magnetic properties of amorphous magnetic materials is perspective direction.

In this work we report on the Monte Carlo simulation of the magnetic properties of pure amorphous Gd and amorphous alloys of the Re-Gd system which are not studied so far.

2. Simulation technique
Using the molecular dynamics method, we constructed the models of atomic structure of pure amorphous Gd and Re-Gd amorphous alloys. Each model contained 100 000 atoms in a cubic cell with periodic boundary conditions. The interatomic interaction was described by an empirical polynomial potential [4].

The magnetic moments of Gd atoms in the process of simulation were situated in the corresponding atomic locations in the amorphous structure. The coordinates of the atoms were previously obtained by the molecular dynamics method. Magnetic properties of these models were studied using the Monte Carlo method within the standard Metropolis algorithm [5] in the framework of the Heisenberg model. After formation of a random initial spin configuration, an attempt of changing the configuration is made, i.e. the randomly chosen spin randomly changes its spherical
coordinates θ and φ. If the energy of the system is decreases after this change, then the new configuration is accepted, otherwise it is accepted with the probability \( W = \exp(-\Delta E/k_B T) \) where \( \Delta E \) is the energy variation. This procedure repeats for calculation of average values of physical quantities.

The Hamiltonian describing the interaction of the magnetic moments of gadolinium atoms was written in the following form [6, 7]:

\[
E = -\frac{1}{2} \sum_{i,j} J_1 (S_i \cdot S_j) - \frac{1}{2} \sum_{i,k} J_2 (S_i \cdot S_k) - \mu H \sum_i S_i^z
\]

where \( J_1 > 0 \) is the exchange interaction integral between the spins \( S_i \) and \( S_j \) within the distances not exceeding \( r_1^{\text{min}} = 0.455 \) nm – the position of the first minimum of the pair RDF \( g(r) \); \( J_2 < 0 \) is the exchange interaction integral between the spins within the distances in the interval from \( r_1^{\text{min}} \) to \( r_2^{\text{max}} = 0.77 \) nm – the first and the second minima of the pair RDF \( g(r) \); \( \mu = 7.98 \mu_B \) is the effective magnetic moment of the Gd atom; \( H \) is the strength of the external magnetic field.

The value of the exchange integral within the first coordination sphere was chosen \( J_1 = 45.7 \) K. The value of the exchange integral within the second coordination sphere \( J_2 \) varied in the following range: \( J_1/|J_2| = 2, 6, 8, 9, 10, 11, 12, 13, 14 \) and 16.

During the cooling process the temperature dependencies of potential energy of the system (1), magnetization \( M(T) \), Edwards–Anderson order parameter \( q(T) \) and magnetic susceptibility \( \chi(T) \) were calculated.

3. Results and discussion

For the model of pure amorphous Gd, we calculated the temperature dependencies of spontaneous magnetization \( M \), where \( M_s \) is saturation magnetization, at various values of the \( J_1/|J_2| \) ratio \( (J_1/|J_2| = 10, 11, 12, 13, 14) \). In the Fig. 1 we present the dependence of maximum spontaneous magnetization (at \( T = 1 \) K) on the \( J_1/|J_2| \) ratio for the model of amorphous Gd.

![Fig. 1. Dependence of maximum spontaneous magnetization (at \( T = 1 \) K) on the \( J_1/|J_2| \) ratio for the model of amorphous Gd](image_url)
As it is seen from Fig. 1, at the low temperatures at \( J_1/|J_2| \geq 13 \) the ferromagnetic state takes place, at \( 11 < J_1/|J_2| < 13 \) – the asperomorphic state, and at \( J_1/|J_2| \leq 11 \) the system transits into the spin-glass state. In the asperomorphic state the spontaneous magnetization differs from zero but the magnetic moments are non-collinear, arranged randomly as in spin glasses. The type of a phase was determined by the value of \( M/M_s \) at \( T = 0 K \).

In Fig. 2 we present the temperature dependencies of magnetic susceptibility for the models of pure amorphous gadolinium at different values of the \( J_1/|J_2| \) ratio equal to 8, 10, 12, 14 and 16. The values of susceptibility were calculated during cooling the model from the paramagnetic state in the temperature interval \( T = 100 \rightarrow 1 K \) with the step \( \Delta T = 5 K \) in the absence of magnetic field. At each temperature the values of susceptibility were averaged over 10 cycles of \( 10^3 \) MC-steps/spin. In all these \( \chi(T) \) curves a distinct maximum is observed that proves the presence of a magnetic phase transition. Position of the maximum corresponds to the phase transition temperature \( T_f \).

![Fig. 2. Temperature dependence of magnetic susceptibility for the model of amorphous Gd at different values of the \( J_1/|J_2| \) ratio](image)

Thus, we obtained the magnetic phase diagram for amorphous Gd in the \( J_1/|J_2| - T \) coordinates (Fig. 3). It allows one to determine the phase state of the system depending on the temperature and the exchange integral within the second coordination sphere \( J_2 \). The temperature of the magnetic phase transition increases monotonically with increasing the \( J_1/|J_2| \) value and reaches the constant value \( T_f \approx 75 K \) at \( J_2 \rightarrow 0 \) (in this case \( J_1/|J_2| \rightarrow \infty \)).

We studied the temperature dependencies of magnetic susceptibility \( \chi(T) \) for amorphous alloys \( \text{Re}_{100-x}\text{Gd}_x \) (\( x = 4, 5, 7, 8, 10, 12, 37, 61 \) and 93 at. %) with \( J_1/|J_2| = 10 \). At \( x > 7 \) at. % Gd in all the \( \chi(T) \) curves the distinct maxima are observed. The temperatures of the spin glass transition \( T_f \) were determined by the positions of the maxima. At \( x \leq 7 \) at. % Gd a maximum in the \( \chi(T) \) curves disappears and magnetic susceptibility monotonically increases with decreasing the temperature, what is typical for paramagnetic state.
Fig. 3. Magnetic phase diagram $T_f(J_1/|J_2|)$ for the model of amorphous Gd

The minimal concentration of gadolinium atoms at which the spin glass transition takes place is above the percolation threshold in this system that is 4 at. % Gd. Thus, the spin glass transition in the Re-Gd system takes place only above the percolation threshold in this system, i.e. at $x > 7$ at. % Gd.

The temperature dependence of the transition temperature (Fig. 4) is linear and agrees well with the experimental results [3].

Fig. 4. Dependence of the spin-glass transition temperature for the models of Re$_{100-x}$Gd$_x$ amorphous alloys on the concentration of Gd atoms

We studied the behaviour of the models of amorphous Gd and Re-Gd amorphous alloys with application of an external magnetic field. The hysteresis loops for the model of amorphous Gd were calculated at $J_1/|J_2|=10$ (this corresponds to the spin-glass state) and temperatures $T=1, 30, 50$ K (Fig. 5). The external magnetic field was varied from $-100$ to $100$ kOe with a step $5$ kOe. The coercive
field at $T=1$ K is $\sim 10$ kOe and the remanent magnetization is $\sim 0.55M_S$. With increasing the temperature, the coercive field and the remanent magnetization monotonically decrease and reduce to zero at the spin-glass transition temperature $T_f = 50$ K.

The hysteresis loops for the models of Re$_{100-x}$Gd$_x$ amorphous alloys at $T=1$ K were also calculated (Fig. 6). The external magnetic field was also varied from $-100$ to $100$ kOe with a step $5$ kOe. At $x = 12$–61 at. % Gd the coercive field is less than $5$ kOe and only at $x = 93$ % it is about $10$ kOe. The remanent magnetization monotonically increases with increasing the concentration of gadolinium atoms.

The results of Monte Carlo simulation of magnetization and remagnetization processes coincide qualitatively with the results of experimental study of various amorphous alloys based on rare-earth metals [8, 9].

![Fig. 5. Hysteresis loops for the model of amorphous Gd at $J_z/|J_z|=10$ and different temperatures](image)

![Fig. 6. Hysteresis loops for the models of Re$_{100-x}$Gd$_x$ amorphous alloys at $T=1$ K](image)
4. References

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