Computer simulation of magnetic properties of Re-Tb amorphous alloys

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Abstract. Using the Monte Carlo method in the frame of the Heisenberg model we performed simulation of magnetic properties of Re\textsubscript{100-x}Tb\textsubscript{x} (x=5–91 at. %) amorphous alloys and of pure amorphous Tb. Exchange interaction between the nearest neighbours and random uniaxial anisotropy were taken into account in the Hamiltonian. We calculated temperature dependence of magnetization, Edwards–Anderson order parameter and magnetic susceptibility. The spin-glass transition temperatures were obtained.

1. Introduction
Spin glasses are of great interest as a new class of magnetic materials having the unique physical properties [1]. In amorphous alloys, as well as in the crystalline materials, competition among exchange interactions can arise which is connected with spatially chaotic atomic arrangement. Besides, in amorphous alloys, because of presence of the topological and compositional disorder, random magnetic anisotropy appears which can also lead to the spin-glass state.

It is known that heavy rare-earth metals (REM) with the non-zero atomic orbital moment have the gigantic magnetic anisotropy [2]. Hence, many of the amorphous alloys of REM with noble, normal and ferromagnetic 3d-metals at low temperatures have the spin-glass properties [3]. Binary amorphous alloys of REM with nonmagnetic transition metals are very little studied, although in this case the transition to the spin-glass state also takes place. In amorphous alloys of the Re\textsubscript{100-x}Tb\textsubscript{x} (x=20–91 at. %) system the typical for spin glasses maximum on the temperature dependence of dynamic magnetic susceptibility $\chi(T)$ and irreversibility of magnetization $M(T)$ were experimentally revealed [4]. The temperature of the phase transition increases linearly when increasing the concentration of magnetic ions.

However, the nature of the state spin glasses with random anisotropy on the microscopic level is studied insufficiently. This encourages one to construct and analyze computer models of atomic structure and magnetic properties of these materials.

2. Computational technique
Using the molecular dynamics method we constructed the models of atomic structure of the Re-Tb amorphous alloys and of pure amorphous Tb in the wide compositional region. Interatomic interaction was described by a model polynomial potential [5]. The detailed description of simulation of atomic structure is given in ref. [6]. Radial distribution functions and parameters of topological short-range...
order calculated for the models are in good agreement with the results of the X-ray diffraction experiment [7].

Using the Monte Carlo method in the frame of the Heisenberg model we carried out simulation of magnetic properties of Re-Tb amorphous alloys and of pure amorphous Tb. The standard Metropolis algorithm was used for the Monte Carlo method [8]. Exchange interaction between the neighbouring magnetic ions and the random magnetic anisotropy play the most important role in forming of the magnetically ordered structures in amorphous alloys containing REM. That is why we used the following model Hamiltonian [9]:

\[
H = -\frac{1}{2} J \sum_{i,j} \left( \hat{S}_i \cdot \hat{S}_j \right) - D \sum_i \left( \hat{n}_i \cdot \hat{S}_i \right)^2 ,
\]

where \( J \) is exchange interaction constant between the pairs of Tb ions; \( D \) is anisotropy constant; \( \hat{S}_i \) is classical Heisenberg spin placed in each site of the model amorphous structure; \( \hat{n}_i \) is unit vector determining the direction of the local anisotropy axes.

Directions of local anisotropy axes were chosen randomly at each site. The value of anisotropy constant is a fitting parameter of the model. The value of exchange interaction constant was chosen equal for all pairs of Tb atoms which are the nearest neighbours and was equal to that for crystalline Tb (\( J = 31.8 \) K) [2].

We performed cooling of the model in the temperature interval \( T = 300 \) K with the step \( \Delta T = 10 \) K or \( \Delta T = 5 \) K and calculated temperature dependencies of the potential energy of the system, spontaneous magnetization \( M(T) \), and the Edwards–Anderson order parameter \( q(T) \) by the formula

\[
q = \frac{1}{N} \sum_i \left( \langle \hat{S}_i \rangle_r \right)^2
\]

where \( N \) is number of Tb atoms; \( \langle \ldots \rangle_r \) is averaging over time during \( 10^7 \) Monte Carlo steps per spin.

We also calculated temperature dependence of magnetic susceptibility \( \chi(T) \) by the formula

\[
\chi = \frac{J N}{kT} \left( \langle M^2 \rangle - \langle M \rangle^2 \right)
\]

3. Results and discussion

For the model of pure amorphous Tb consisting of 30000 atoms we calculated the temperature dependencies of magnetization (figure 1) and the Edwards–Anderson order parameter at different values of ratio of the anisotropy constant to the exchange constant \( D/J \). In all the calculations the value of the Edwards–Anderson order parameter tends to unity when \( T \rightarrow 0 \) which is evidence of the presence of magnetically ordered phase for all the values of \( D/J \) being considered. Analyzing the \( M(T) \) curves, we can conclude that at \( D/J=0 \) the ferromagnetic ordering takes place in the system. Considering the \( D/J=1, 8, 15 \) and 20 - the asperomagnetic ordering, and at \( D/J=10^2 \) - speromagnetic ordering, which is characteristic for the spin glasses with high concentrations of the REM atoms [11].

The temperature of magnetic phase transition was determined as the position of peaks on temperature dependencies of magnetic susceptibility (figure 2). The values of susceptibility were obtained during cooling of the model, and at each temperature the values were averaged over 10 cycles of \( 3 \times 10^7 \) Monte Carlo steps. The temperature of magnetic ordering is the same for all \( D/J \) values and lies between 110 and 120 K, and it slightly increases with increasing the \( D/J \) value.

We also studied magnetic properties of the models of Re_{100-x}Tbx (x=5, 8, 10, 13, 20, 29, 49, 59 and 91 at. %) amorphous alloys consisting of 30000 atoms. As it is known, with increasing of concentration of Tb atoms in the alloy, the random anisotropy constant also increases [10]. Therefore we chose the random anisotropy constant for the alloys linearly dependent on the concentration of Tb atoms: \( D/J = 30 \cdot x/100 \). In all the models the transition to the spin-glass state was observed except of
Re$_{95}$Tb$_5$ amorphous alloy where paramagnetic phase exists in the entire temperature region up to 1 K. Magnetization at low temperatures for all compositions did not exceed 0.1. The temperature of the spin-glass transition was determined as position of maximums on temperature dependencies of magnetic susceptibility (figure 3). With increasing concentration of Tb atoms the transition temperature linearly increases, this linear dependence qualitatively agrees with the experimental results (figure 4).

Difference between the model and experimental temperatures of the spin-glass transition is probably caused by the fact that the exchange interaction constant in amorphous state is smaller than that in crystalline phase. As a first approach, we chose this value equal to that in the crystalline terbium. As the additional calculations showed, the transition temperature is mainly determined by the value of the exchange interaction constant and very slightly depends on the anisotropy constant. With $J=0$ and even very high values of $D$ no phase transition was observed, the model remained paramagnetic at all the temperatures. Therefore, selection of the proper value of the exchange constant can bring the model values of the transition temperatures to agreement with the experimental ones.

**Figure 1.** Temperature dependencies of spontaneous magnetization for the model of pure amorphous Tb (30000 atoms) with different values of anisotropy constant.

**Figure 2.** Temperature dependence of magnetic susceptibility for the model of pure amorphous Tb with different values of anisotropy constant.
Figure 3. Temperature dependence of magnetic susceptibility for the models of Re_{100-x}Tb_x amorphous alloys.

Figure 4. Dependence of the spin-glass transition temperature on the composition of the Re-Tb amorphous alloys.

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