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# Spin glass transition in canonical AuFe alloys: A numerical study

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ABSTRACT

Although spin glass transitions have long been observed in diluted magnetic alloys, e.g. AuFe and CuMn alloys, previous numerical studies are not completely consistent with the experiment results. The abnormal critical exponents of the alloys remain still puzzling. By employing parallel tempering algorithm with finite-size scaling analysis, we investigated the phase transitions in canonical AuFe alloys. Our results strongly support that spin glass transitions occur at finite temperatures in the alloys. The calculated critical exponents agree well with those obtained from experiments.



## 1. Introduction

Despite decades of research, spin glass (SG) is still one of the most active subjects which attracts extensive attention [1,2]. So far, SG phases have been verified in many disordered magnetic systems [3–7] and become already the fundamental states of magnetism. Among various SG materials, AuFe and CuMn alloys with low concentrations of magnetic impurities, have long been used to explore different SG properties [8,9]. In these alloys, magnetic impurities interact with each other via the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction. This interaction oscillates in real space with alternate ferromagnetic and antiferromagnetic coupling and may result in magnetic frustration, which is the key factor to lead to spin glass phase.

Nevertheless, several problems on canonical SGs still remain puzzling, i.e., the measured non-Ising critical exponents [10], the mean-field-like transition in magnetic field [11,12], the absence of the Heisenberg-to-Ising crossover in nonlinear susceptibility [10]. Although spin glass transitions have long been observed in canonical SGs [13,14], theoretical studies are not completely consistent with the experimental results. For instance, some earlier simulations did not find a SG transition in the AuFe alloy using a RKKY model without anisotropy [15,16]. Matsubara and Iguchi demonstrated that a SG transition occurred in the metallic alloys at finite temperature [17], but their simulations suffered from poor sample averages. Some first-principles studies also showed that less frustration existed in AuFe alloy with increasing impurity concentrations [18]. Moreover, the critical exponents obtained from those numerical simulations did not agree with the experimental results. Indeed, the critical exponents experimentally measured for typical canonical SG materials range with $\nu \simeq 1.3 \sim 1.4$ and $\eta \simeq 0.4 \sim 0.5$ [19–24], while the values from numerical simulations yield $\nu \simeq 2.5 \sim 2.7$, $\eta \simeq -0.38 \sim -0.40$ for the $\pm J$ and bimodal Ising model [25,26] and $\nu = 1.49$, $\eta = -0.19$ for the Heisenberg Edwards–Anderson (EA) model [27]. Therefore, the critical exponents obtained from experiments cannot be assigned to Heisenberg-type or Ising-type. It is even proposed that the abnormal critical exponents are caused by an occurrence of chiral-glass (CG) transition in the alloys [11,19]. But this suggestion also raises two other problems: (i) the chirality must couple to the spins via magnetic anisotropy [11], which does not exist in canonical SGs; (ii) the critical exponents of chirality obtained from site-regular models do not correspond to the site-disordered case in real alloys. Up to now, these problems are still unsolved and require further clarification.

In this Letter, we report our theoretical investigation on the phase transitions in canonical AuFe SGs. Using parallel tempering algorithm [28,29] combined with the heat bath method [30,31], we calculate the SG correlation lengths and the nonlinear susceptibility in AuFe alloys for two impurity concentrations. By finite-size scaling we find that SG transitions do occur in the alloys at finite temperatures. The critical exponents $\nu$ and $\eta$ obtained from our simulations agree well with those from experiments [19–24].

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## 2. Model, methods and quantities

We use a face-centered cubic (FCC) lattice to study the SG transitions for AuFe alloys. The lattice sizes are set to be 5, 6, 7 and 8. Spins randomly occupy the sites and two spin concentrations of $c = 8\%$ and 12% are investigated in the simulations. We consider only the RKKY interactions between spins and omit the direct exchange coupling which rarely occurs in real SG alloys. Hence, the Hamiltonian of the interacting spins can be written as

$$H = \sum_{i,j} J(r_{ij})\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \tag{1}$$

$$J(r_{ij}) = J_0\left[\frac{\cos(2k_F r_{ij})}{(2k_F r_{ij})^3} - \frac{\sin(2k_F r_{ij})}{(2k_F r_{ij})^4}\right] \tag{2}$$

where $J_0$ is the coupling constant and $\boldsymbol{\sigma}$ is a unit spin vector rotating in space. For convenience the temperature takes the unit of $J_0/k_B$, which is set to be 1.0 in our simulations. $k_F$ is the Fermi-wave vector and set to be $2\pi/(5a)$, where $a$ is the lattice constant. The $k_F$ value is close to the one obtained from the first-principles calculations on AuFe alloys [18]. The periodical boundary conditions are employed in our simulations. We use the heat bath method [30,31] to update the spin configurations. The parallel tempering method [28,29] is used to efficiently speed up the thermalization of the system replicas, which have identical parameters but evolve independently. The differences of inverse temperature for the nearest replicas, $\Delta\beta$, are carefully chosen to make sure that the exchange occurs frequently even at low temperature. Actually, we set $\Delta\beta = 4.0$ for the case of concentration $c = 8\%$ and $\Delta\beta = 3.0$ for the case of $c = 12\%$. In this way, more replicas are distributed at lower temperatures to ensure that the replicas exchange their configurations frequently.

Generally, when a matter undergoes continuous phase transition, its order emerges and the correlation length diverges at the critical temperature. For a SG system, its order parameter is defined as the spin overlaps between two replicas [25–27]. As temperature decreases below the critical temperature, the spins in SGs become frozen and the relative directions between two spins are nearly constant, and the correlation length increases significantly, or in other words, the system goes into SG phase. In most simulations, by scaling the correlation lengths, a SG phase transition can be detected accurately [25–27,32–34]. The components of the wave-vector dependent SG order parameter can be written as

$$q_{\mu\nu}(\boldsymbol{k}) = \frac{1}{N}\sum_r \sigma_\mu^\alpha \sigma_\nu^\beta e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{3}$$

where $\mu$ and $\nu$ ($\mu, \nu = x, y, z$) are the spin components along three dimensions, $\boldsymbol{r}$ is the position vector of the selected spin, $\alpha$ and $\beta$ are the replica indices. Thus the $k$-dependent order parameter of spin glass can be defined as

$$q(\boldsymbol{k}) = \sqrt{\sum_{\mu,\nu} \left|q_{\mu\nu}(\boldsymbol{k})\right|^2}. \tag{4}$$

The nonlinear SG susceptibility is defined as $\chi_L(0) = N[\langle q(\boldsymbol{k} = 0)^2\rangle]$, where the angle brackets and square brackets mean that the thermal and disordered averages are taken respectively.

Usually, Binder ratios are calculated to indicate whether the system undergoes a SG transition. The size-dependent Binder ratio is defined as in [25,32]

$$B_L = \frac{1}{2}\left(3 - \frac{[\langle q^4(0)\rangle]}{[\langle q^2(0)\rangle]^2}\right). \tag{5}$$

However, recent studies on the site-disordered SGs reported that the scaling corrections of the Binder ratios were very large [32], and in some cases they did not cross at all [27,34]. Fortunately, an elegant method based on the scaling of finite-size correlation lengths was developed and widely used in the recent simulations [33,34]. In this method, the finite-size correlation length of the spin glass, $\xi_L$, is used, which can be expressed as

$$\xi_L = \frac{1}{2\sin(k_{\min}/2)}\sqrt{\frac{\chi(0)}{\chi(\boldsymbol{k}_{\min})} - 1}, \tag{6}$$

where $\boldsymbol{k}_{\min} = (2\pi/a, 0, 0)$ or its permutations. The correlation lengths are expected to satisfy the conventional scaling relation [33]

$$\xi_L/L = F\left[(L)^{1/\nu}(T - T_g)\right]. \tag{7}$$

If the system undergoes a spin glass transition, all the correlation lengths with different sizes are expected to make a common crossing at $T = T_g$.

Note that all the quantities mentioned above must be measured after the systems have been relaxed into equilibrium states. Due to frustration and disorder in SG system, one must overcome the critical slowing down problem to relax the SG into equilibrium. Thanks to the emerging powerful algorithms, i.e. the parallel algorithm [28,29] and heat bath sampling [30,31], an equilibrium state can be reached in SG simulations [25–27]. Currently, both methods are widely used in SG simulations to investigate the equilibrium properties [33,34]. Experimentally, the slow-relaxing phenomena were also observed by different measuring protocols. For instance, a critical temperature increases with increasing field frequency in magnetic measurements [1,35,36]. For current simulations on equilibrium states, the situation must correspond to the quasistatic process in experiments, e.g. a slow cooling rate for samples and a DC measuring mode with minute-scale for each data collecting. We assume the systems have reached equilibrium when the correlation length at the lowest temperature becomes saturated with increasing Monte Carlo sweeps. In practice, the equilibrium can be recognized by plotting the logarithmic Monte Carlo steps versus the correlation length. By preliminary calculations, we extract the necessary Monte Carlo sweeps and list them together with other parameters in Table 1. Due to the RKKY long-range interactions, the calculation complexity increases proportionally to $L^6$, which forbids us to calculate larger systems. The FCC lattice employed in our simulations also contains four times as many spins as those in the simple cubic lattice of the same size. The largest system we can equilibrate is the case of $L = 8$ with $c = 12\%$, which contains about 246 spins. The simulations are extremely time-consuming and totally $1 \cdot 10^5$ CPU hours are cost to generate the present results.

**Table 1**
The parameters used in the simulations. $L$ is the linear size of the system. $N_s$ is the average spins contained in the simulation system. $N_{\text{av}}$ is the number of configurations for disorder average. $N_e$ is the sweeping number needed to equilibrate the replicas. We use $N_m$ sweeps to collect data for calculating the quantities. Totally, 38 replicas are used for the case of 8% and 44 replicas for the case of 12%. $T_{\max}$ and $T_{\min}$ are the highest and lowest temperatures, respectively.

| $L$ | $N_s$ | $N_{\text{av}}$ | $N_e$ | $N_m$ | $T_{\min}$ | $T_{\max}$ |
|---|---|---|---|---|---|---|
| $c = 8\%$ | | | | | | |
| 5 | 40 | 2600 | $6 \cdot 10^5$ | $6 \cdot 10^5$ | 0.007 | 0.032 |
| 6 | 69 | 2000 | $8 \cdot 10^5$ | $8 \cdot 10^5$ | 0.007 | 0.032 |
| 7 | 109 | 1600 | $1.2 \cdot 10^6$ | $8 \cdot 10^5$ | 0.007 | 0.032 |
| 8 | 164 | 1000 | $2 \cdot 10^6$ | $1 \cdot 10^6$ | 0.007 | 0.032 |
| $c = 12\%$ | | | | | | |
| 5 | 60 | 2200 | $8 \cdot 10^5$ | $6 \cdot 10^5$ | 0.0094 | 0.048 |
| 6 | 104 | 1600 | $1 \cdot 10^6$ | $8 \cdot 10^5$ | 0.0094 | 0.048 |
| 7 | 165 | 1200 | $1.6 \cdot 10^6$ | $1 \cdot 10^6$ | 0.0094 | 0.048 |
| 8 | 246 | 800 | $2.4 \cdot 10^6$ | $1 \cdot 10^6$ | 0.0094 | 0.048 |