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To cite this version:

Y. Kakehashi. ITINERANT-ELECTRON SPIN GLASS IN IRON-BASE ALLOYS. Journal de Physique Colloques, 1988, 49 (C8), pp.C8-1079-C8-1080. <10.1051/jphyscol:19888494>. <jpa-00228699>

HAL Id: jpa-00228699
https://hal.archives-ouvertes.fr/jpa-00228699
Submitted on 1 Jan 1988

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ITINERANT-ELECTRON SPIN GLASS IN IRON-BASE ALLOYS

Y. Kakehashi

Department of Physics, Hokkaido Institute of Technology, Teine-Maeda, Nishi-ku, Sapporo 006, Japan

Abstract. – On the basis of the numerical calculations for the fcc Fe-Ni alloys, we have shown that the close-packed Fe alloys form a new type of itinerant-electron spin glass because of the non-linear magnetic coupling between Fe local moments and the local environment effect on the amplitude of Fe local moments.

Quite recently the spin glass (SG) state has been found in the fcc (Fe$_{25}$Ni$_{75}$)$_{92}$C$_8$ [1], Fe$_{80}$Ni$_{20}$Cr$_{20}$ [2], Fe-Zr amorphous [3], and Fe-La [4] amorphous alloys. The close-packed Fe alloys mentioned above are typical itinerant-electron systems because of the following reasons, and therefore form a new family of the itinerant-electron SG. First the effective Bohr magneton number of $\gamma$Fe(7 $\mu_B$) is ten times as large as the ground-state sublattice magnetization (0.7 $\mu_B$). Thus the Rhodes-Wohlfarth ratio [5] is much larger than the value (= 1) obtained from the localized model. Second the specific heat anomaly in Fe-Ni alloys becomes very small near the critical concentration of the ferromagnetic instability [6]. This implies very small magnetic entropy in contradiction to that expected from the simple localized model (i.e. $\sum \alpha$ ln (2$S_{\alpha}$ + 1), $S_{\alpha}$ being the concentration of the atom $\alpha$ with the localized spin $S_{\alpha}$).

In this presentation we argue the theoretical aspect of these itinerant-electron SG on the basis of the numerical calculations of the magnetic phase diagram in the fcc Fe-Ni alloys.

The calculations are based on the finite-temperature theory of the local environment effect [7]. The theory reduces to the interpolation theory developed by Hubbard and Hasegawa [8] in the pure metal limit. In alloys the theory selfconsistently takes into account a large number of magnetic and atomic configurations on the surrounding atoms (e.g. 16777216 for the fcc and 65536 for the bcc) by means of the method of distribution function [8], therefore describes the metallic SG. In particular the SG temperature $T_g$ reduces to the wellknown formula of the molecular field approximation with the Anderson superexchange interactions in the insulator limit.

We show in figure 1 the calculated phase diagram of Fe-Ni alloys which are regarded as a prototype of the itinerant electron SG. The present theory certainly leads to the SG state after disappearance of the ferromagnetism. Calculated susceptibilities show a clear cusp at $T_g$ and follow the Curie-Weiss law at higher temperatures. The concentration dependence of $T_g$ seems to be consistent with the experimental results for (Fe$_{25}$Ni$_{75}$)$_{92}$C$_8$ [1]. The absolute values ($\sim$ 150 K) are however several times higher than the experimental values ($\sim$ 30 K [1]). The overestimate of $T_g$ is probably due to the molecular field approximation. The strong frustration effect is expected in the (Fe$_{25}$Ni$_{75}$)$_{92}$C$_8$ and Fe$_{80}$Ni$_{20}$Cr$_{20}$ because of the antiferromagnetic interactions on the fcc lattice. This is confirmed by comparing $T_g$ (30 K) in (Fe$_{25}$Ni$_{75}$)$_{92}$C$_8$ [1] and Fe$_{80}$Ni$_{20}$Cr$_{20}$ [2] with those ($\approx$ 120 K) in amorphous Fe$_{95}$Zr$_7$ [3] and Fe$_{80}$La$_{20}$ [4] alloys in which the magnetic frustration inherent in the fcc lattice must be removed.

An important point is that the existence of the SG can not be explained by a simple localized model because all the calculated effective exchange interactions $J_{\alpha\gamma}$ in Fe-Ni alloys are positive (i.e. ferromagnetic) in the spin glass regime. We examined therefore the adiabatic exchange pair energy in an effective medium as a function of the amplitude of the central local moment (LM) when the neighboring LM points up, and found that the magnetic coupling between Fe LM shows an anomalous nonlinearity; the Fe LM with the amplitude larger than about 1.7 $\mu_B$ favor the ferromagnetic coupling to the neighboring Fe LM, while those with the amplitude smaller than 1.7 $\mu_B$ favor the antiferromagnetic couplings. On the other hand the amplitude of LM is determined by the local environment i.e.
the surrounding atomic configuration. The increase of the number of surrounding Fe atoms decreases the amplitude of the central Fe LM. In the local environments with more than 10 Fe nearest neighbors the Fe LM have their amplitudes smaller than about 1.7 \( \mu_B \), therefore antiferromagnetically couple to the neighboring Fe LM, but in the environment with less than 10 Fe nearest neighbors the Fe LM have the amplitude larger than 1.7 \( \mu_B \), thus show the ferromagnetic coupling to the neighboring Fe LM (See Fig. 2). These ferro-and antiferro-magnetic couplings between Fe LM cause the SG in Fe-Ni alloys. The mechanism is based on the nonlinearity of the magnetic coupling between Fe LM and the local environment effect on the amplitude of Fe LM, which are never seen in the localized model. Thus the SG in the fcc Fe-Ni alloys belong to a new type of itinerant-electron SG. We also performed the theoretical calculations for the fcc Fe-Co alloys, and found that the SG appears after disappearance of the ferromagnetism at 80 at \% Fe. The mechanism for the formation of the SG is just the same as in the Fe-Ni alloys. The same mechanism is also expected in the amorphous Fe-Zr and Fe-La alloys because recent first principle calculations [10] show that the density of states for nonmagnetic amorphous Fe is rather close to the \( \gamma \)Fe.

We emphasize that the origin of the SG mentioned above has also explained the rapid deviation from the Slater-Pauling curves and the temperature dependence of the broad internalfield distribution near the critical concentration of the ferromagnetic instability in Fe-Ni alloys [7].

In conclusion we have demonstrated that the SG in the fcc Fe-Ni and Fe-Co alloys are theoretically possible, and they are new type of itinerant-electron SG. We speculate that the SG in the amorphous Fe alloys are also based on the same mechanism. In particular we believe that the ground state of amorphous Fe is the SG. Theoretical calculations for our speculation are in progress.

Fig. 2. – Nonlinear coupling between Fe LM’s in the fcc Fe alloys. Fe LM’s with less than 10 Fe nearest neighbors have large amplitudes, therefore show the ferromagnetic coupling. But Fe LM’s with more than 10 Fe nearest neighbors have small amplitudes, thus the antiferromagnetic coupling.

\[ \text{Fe} \Downarrow \overline{\text{Fe}} \] 
\[ \text{Fe} \Downarrow \overline{\text{Fe}} \] 
\[ \text{Fe NN} \geq 10 \] 
\[ \text{Fe NN} \leq 10 \]