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1992 J. Phys.: Condens. Matter 4 L339

(http://iopscience.iop.org/0953-8984/4/24/001)

J. Phys.: Condens. Matter 4 (1992) L339–L344. Printed in the UK

LETTER TO THE EDITOR

The spin distribution of a plastically deformed Pt_3Fe single crystal

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Received 13 April 1992

Abstract. The magnetization curves of a plastically deformed Pt_3Fe single crystal were measured, applying the external field in three orthogonal directions [110], [$\bar{1}$10] and [001], in the temperature range from 77 K to room temperature. The spontaneous magnetization M_s, is anisotropic; M_s along [001] is smaller than that along [110] and [$\bar{1}$10] below 180 K, and above 180 K they are isotropic. The ferromagnetism is referred to the atomic rearrangement in the antiphase boundary (APB) between superpartial dislocations; Fe–Fe atom pairs along the APB are located at the first-nearest neighbour positions with a two-dimensional distribution. The three-dimensional values of M_s give information about the spin distribution of Fe atoms near the APB; the spin orientation of the ferromagnetic couplings or the easy axis of magnetization is one of the $\langle 100 \rangle$ directions that is perpendicular to the Burgers vector of the superpartial dislocations.

Pt_3Fe crystal has an $L1_2$-type atomic structure and antiferromagnetic structure (Crangle 1959, Bacon and Crangle 1963); below 100 K the magnetic structure is characterized by the wave vector $(2\pi/a)(\frac{1}{2}, 0, 0)$, in which Fe moments of 3.3 μ_B are aligned ferromagnetically on (100) subsheets, and between 100 K and 170 K the wave vector is $(2\pi/a)(\frac{1}{2}, \frac{1}{2}, 0)$ and the ferromagnetic subsheets are (110). Here a is a lattice parameter. In plastically deformed Pt_3Fe crystal a remarkable magnetic transition to ferromagnetism was discovered by Bacon and Crangle (1963). The mechanism of the magnetic transition was elucidated in terms of superlattice dislocations from the viewpoint of a localized electron model (Takahashi and Ikeda 1983). The magnetic moments of Fe atoms are ferromagnetically coupled in the vicinity of the antiphase boundary (APB) between superpartial dislocations. This idea was confirmed experimentally and a few phenomena have been found that are difficult to explain on the basis of the localized electron model (Takahashi and Umakoshi 1990): (i) along the APB, Fe atoms couple ferromagnetically and exert a magnetic influence on the neighbouring Fe atoms up to 10 nm away; (ii) the spontaneous magnetization, M_s, takes a local maximum near the Néel temperature. It is of interest to us to investigate whether the localized electron model is effective in explaining the magnetic structure in Pt_3Fe alloy.

The magnetic moments coupled ferromagnetically as well as antiferromagnetically would be oriented in $\langle 100 \rangle$ directions; the easy axis of magnetization would be in the $\langle 100 \rangle$ direction in the plastically deformed Pt_3Fe alloy according to Bacon and Crangle (1963). It is obscure, however, whether the spin orientation has three- or two-dimensional symmetry, since the ferromagnetic Fe atoms have a two-dimensional distribution along the {111} APB. It is the purpose of the present study to investigate the spin distribution near the APB, i.e. the geometrical relation between the spin orientation and the slip system.

In the present study, the magnetization was measured while applying a magnetic field to the three orthogonal directions in the Pt_3Fe single crystal. Three-dimensional values of M_s and the magnetic susceptibility have been obtained and the spin orientation near the APB is determined in connection with the Burgers vector of the superpartial dislocations.

Rectangular prisms (50 mm × 3 mm × 3 mm) were cut from a single-crystal rod. They were annealed at 1300 K for one day in vacuum and then cooled very slowly at the rate of 30 K per day to 870 K to obtain a high degree of $L1_2$-type long-range order. The specimen was tested in tension by applying 22% strain at room temperature with an Instron-type machine. The stress axis is near the [110] direction. A cubic specimen was cut from the deformed specimen by spark machining; its faces were oriented at [110], [$\bar{1}$10] and [001]. Magnetic measurements were carried out at temperatures from 77 K to room temperature while applying the magnetic field along the three directions [110], [$\bar{1}$10] and [001].

Magnetization curves were obtained on a balance suitable for measuring the susceptibility of paramagnetic specimens at temperatures from 77 K to room temperature. No significant variation in the susceptibility with magnetic field was detected in the undeformed specimens, implying that no ferromagnetic state was present. The upper and lower panels of figure 1 show the magnetization curves of the specimen plastically deformed by 22% strain with the magnetic field applied in the [110] and [001] directions, respectively. Since even in a magnetic field of 1×10^6 A m^{-1} the magnetization along the [001] direction has a smaller value than that along the [110], there is strong magnetic anisotropy in the ferromagnetic state, with the hard direction of magnetization being [001]. The magnetization deviates from linearity in the low-field range. The susceptibility is obtained from the linear part of the magnetization curves above 4.4×10^5 A m^{-1}. The value of M_s is obtained by the usual procedure of extrapolating the linear part of the magnetic isotherms back to zero magnetic field. The spontaneous magnetizations along the [110], [$\bar{1}$10] and [001] directions are represented as M_s^{110}, $M_s^{\bar{1}10}$ and M_s^{001}, respectively.

The variation in M_s with temperature are shown in figure 2. The values of M_s^{110} and $M_s^{\bar{1}10}$ remain the same over the whole temperature range, but below 150 K, M_s^{110} (or $M_s^{\bar{1}10}$) is larger than M_s^{001}. Above 180 K, M_s takes the same value in the three directions. The temperature dependence is quite different in M_s^{100} and M_s^{001} below 180 K; M_s^{110} (or $M_s^{\bar{1}10}$) decreases rapidly with increasing temperature and the decrease becomes relaxed at 170 K, while M_s^{001} decreases very slowly and takes a local maximum at 170 K. The different temperature dependences suggest the existence of two ferromagnetic states or an anisotropic thermal spin fluctuation.

The reciprocal susceptibility is also plotted against the test temperature in figure 3, which does not follow the Curie–Weiss law. The anisotropy of the susceptibility was clearly observable, especially below 180 K. The rougher variations of the susceptibility could be observed at 100 K, 170 K, 240 K and 260 K.

The magnetic transition due to plastic deformation is attributed to the atomic rearrangement in the APB (Takahashi and Ikeda 1983, Takahashi and Umakoshi 1990). Fe atoms are located at the second-nearest neighbour (NN) in the atomically ordered state, while in the APB, Fe atoms arrange at the first NN along the glide plane; in the APB, there exist Fe–Fe atom pairs with the ⟨110⟩ direction. The direction of these

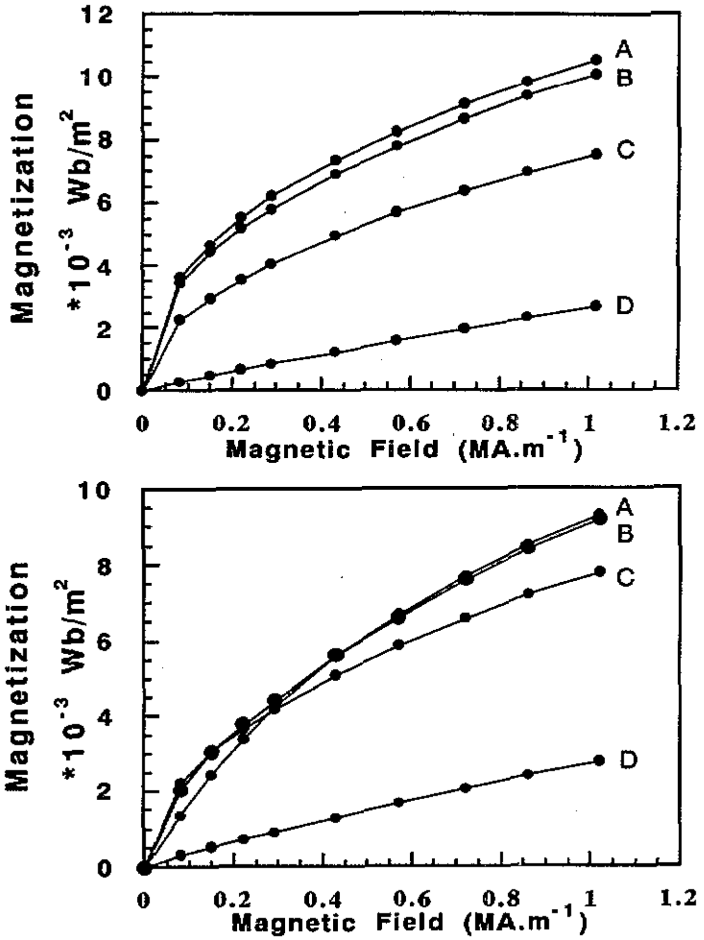

Figure 1. The variation of the magnetization for the 25.6 at.% Fe–Pt alloy elongated by $\epsilon = 22\%$ in the [110] direction with the applied magnetic field in the (upper panel) [110] or (lower panel) [001] direction. The test temperatures are (A) 77 K, (B) 106 K, (C) 160 K and (D) 273 K.

atom pairs depends on the Burgers vector of superpartial dislocations, constituting the APB. The number of Fe–Fe atom pairs can be represented by a simple function of dislocation density, ρ. These Fe–Fe atom pairs would produce the ferromagnetism (Takahashi and Ikeda 1983, Takahashi and Umakoshi 1990). The spin orientation or the easy axis of magnetization would be perpendicular to the pair direction because the dipole–dipole interaction energy becomes a minimum. At the same time the spin orientation should be one of the $\langle 100 \rangle$ directions (Bacon and Crangle 1963).

The tensile direction of the present specimen is near the [110] direction. The possible Burgers vectors being contributed to plastic deformation would be $(a/2)[101]$, $(a/1)[\bar{1}01]$, $(a/2)[011]$ and $(a/2)[0\bar{1}1]$. In the APB between superpartial dislocations, for example, whose Burgers vector is $(a/2)[101]$, the direction of the Fe–Fe atom pairs is $[\bar{1}01]$. Then the spin orientation is [010]. The superpartial dislocations with $(a/2)[011]$ or $(a/2)[0\bar{1}1]$ as the Burgers vector produce ferromagnetic coupling with a [100] spin orientation. Therefore the [001] direction should be the difficult axis of magnetization in the present specimen.

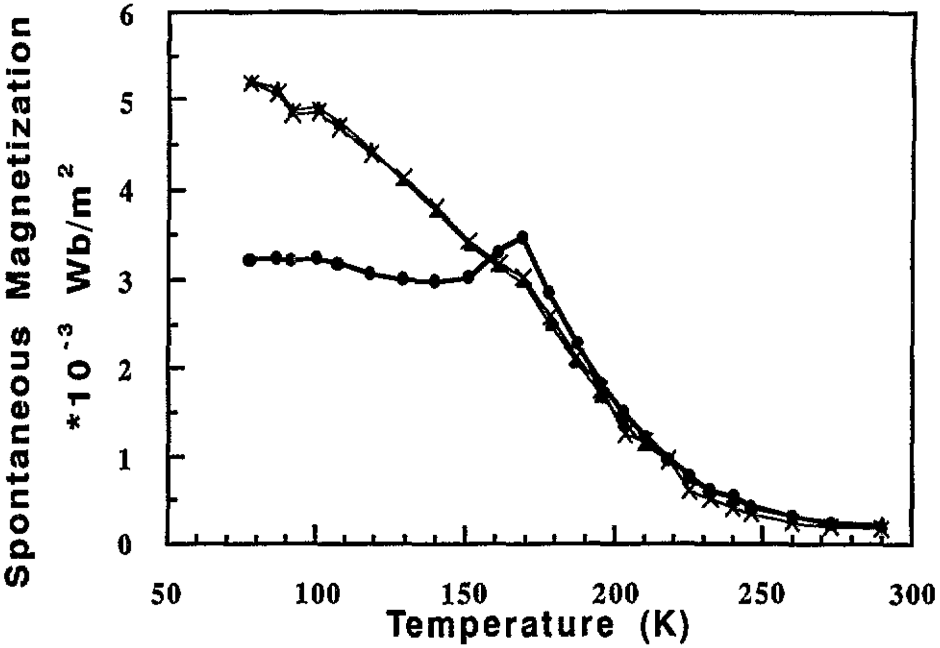

Figure 2. The variation in the spontaneous magnetization with temperature: the applied field is along [110] (▲), [$\bar{1}$10] (×) and [001] (●).

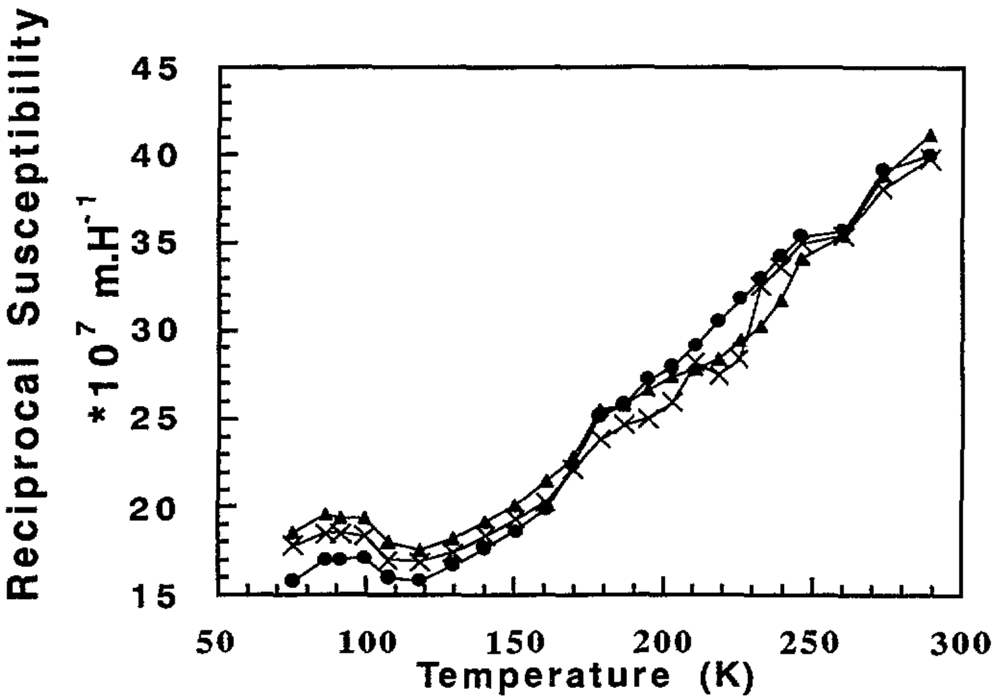

Figure 3. The variation in reciprocal susceptibility with temperature: the applied field is along [110] (▲), [$\bar{1}$10] (×) and [001] (●).

The value of M_s could easily be calculated as a function of ρ and has been compared with the experimental results. The experimental values are more than 10 times as large as the calculated ones. The Fe–Fe atom pairs magnetically enhance the neighbouring Fe atoms and make them ferromagnetic (Takahashi and Umakoshi 1990). The value of ρ in the present specimen was also measured using the electron microscope, and it was found that $\rho = 9 \times 10^9$ cm^{-2}. The long-distance magnetic influence should be considered in the present specimen; Fe–Fe atom pairs separated by 10 to 20 atomic distances from the APB would behave ferromagnetically. Naturally the influence would become weak as the distance increases.

The ferromagnetic spins far from the APB would follow the external field easily in the magnetic measurement. Fe atoms near the APB would have strong uniaxial anisotropy; the first-NN Fe–Fe atom pairs spread along the {111} glide plane. Only one of the ⟨100⟩ directions is the easy axis of magnetization and the anisotropy is uniaxial. The magnetization along [001] does not have the same value as that along [110] and [$\bar{1}$10] in a magnetic field of 1×10^6 A m^{-1} (see figure 1), which suggests that the magnetic anisotropy is very strong. It is, for example, stronger than the magnetocrystalline anisotropy of Fe and Ni crystals.

The value of M_s has been observed along three orthogonal directions. M_s^{110} and $M_s^{\bar{1}10}$ are both larger than M_s^{001}, below 170 K. The ferromagnetic spin distribution in the vicinity of the APB does not contribute to the value M_S^{001}, since spin orientations in the vicinity of the APB are [100] and [010] and the uniaxial anisotropy would be very strong. The value of M_s^{001} would be referred to the magnetization of the neighbouring Fe atoms of the APB that are magnetically enhanced.

The temperature dependence of M_s is different below 170 K; M_S^{110} decreases rapidly with increasing temperature, while M_S^{001} decreases very slowly. The different temperature dependence suggests that the spin distribution in the vicinity of the APB is sensitive to temperature but the ferromagnetic spin distribution away from the APB is not sensitive below 170 K.

M_s^{001} takes a local maximum near 170 K and M_s^{110} and $M_s^{\bar{1}10}$ display relaxation near 170 K in their decrease. The mean distance of superlattice dislocations or APB strips would be 30 nm and there remains antiferromagnetic coupling far from the APB. The antiferromagnetic coupling would change abruptly to ferromagnetic near the Néel temperature, 170 K. Fe atoms, whose spins change from antiferromagnetic to ferromagnetic, would be located at 20 atomic distances from the APB, i.e., at the boundary of the ferromagnetic state and the antiferromagnetic state. The experimental fact that the size of the local maximum increases with increasing ρ is consistent with the present idea (Takahashi and Umakoshi 1990).

The temperature dependence of the reciprocal susceptibility does not show a smooth change; one must acknowledge roughness at 100 K, 170 K, 240 K and 260 K. The temperatures of 100 K and 170 K correspond to the Néel temperatures and 240 K and 260 K would be the Curie temperatures. The recovery process of the magnetic transition due to plastic deformation has been investigated by the present authors (Takahashi and Takahashi 1992), and three recovery processes have been found; M_s decreases in 473 K and 673 K annealing and disappears in 1073 K annealing. The three recovery processes indicate that there exist different ferromagnetic states, i.e. the ferromagnetic coupling of the first-NN Fe atoms in the APB and that enhanced magnetically away from the APB. A ferromagnetic state whose Curie temperature is higher than room temperature has been observed (Bacon and Crangle 1963, Takahashi and Takahashi 1992).

The roughness of the variation of the reciprocal susceptibility indicates the coexistence of antiferromagnetism and ferromagnetism in the plastically deformed Pt_3Fe crystal. Generally, the localized moment model is unable to give a reasonable explanation for the coexistence of ferromagnetic and antiferromagnetic ordered states (Moriya and Usami 1977).

A detailed study is in progress.

References

Bacon G E and Crangle J 1963 *Proc. R. Soc.* A **272** 387
Crangle J 1959 *J. Physique* **20** 435
Moriya T and Usami K 1977 *Solid State Commun.* **23** 935
Takahashi S and Ikeda K 1983 *J. Phys. Soc. Japan* **52** 2772
Takahashi S and Takahashi Y A 1992 *J. Phys.: Condens. Matter* **4** L21
Takahashi S and Umakoshi Y 1990 *J. Phys.: Condens. Matter* **2** 2133