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The commensurate–incommensurate SDW phase boundary of CrFe alloys

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Abstract. The magnetic phase boundary of the commensurate–incommensurate spin density wave (SDW) transition in CrFe alloys was determined more precisely using neutron diffraction of single crystals. The re-entrant incommensurate SDW phase recently reported in CrFeMn ternary alloys was not observed in CrFe binary alloys.

1. Introduction

An incommensurate spin density wave (ISDW) in Cr is very sensitive to alloying and is explained by the nesting Fermi surface model based on the improved rigid-band approximation, which assumes a contribution from the electron reservoirs [1]. Typical alloys are CrMn and CrV systems. In the former, in which Mn is considered as an electron donor, an introduction of a small amount of Mn raises the Néel temperature (T_N) and elongates the wavelength of the SDW. The introduction of only 0.5 at.% Mn changes the ISDW state to a commensurate antiferromagnetic state. On the other hand, alloying with V, which behaves as an electron acceptor, lowers the T_N and shortens the wavelength of the SDW. The CrV alloys including more than 4 at.% V are non-magnetic. However the phase diagram of CrFe alloy, in which Fe is expected to be the electron donor, is different from these typical cases. The wavelength of the SDW behaves like the CrMn alloys with increasing Fe concentration, but the T_N decreases as in the CrV case. In contrast to most of the Cr alloys, the commensurate antiferromagnetic phase (AF_0) is located at a lower temperature than the ISDW phase (AF_1) in CrFe alloy. Thus, the rigid-band description seems to fail for the CrFe alloys. These interesting behaviours in CrFe alloys have lead to several theoretical challenges [2]. Furthermore, Fawcett and Galkin recently reported the existence of the re-entrant incommensurate phase (RAF_1) for CrFeMn ternary alloys [3]. In spite of its importance, however, the magnetic phase diagram of CrFe alloys still includes some ambiguities, especially as to the AF_1–AF_0 phase boundary. A Cr–1.5% Fe alloy is located at a significant position of the phase diagram, but neutron diffraction data at this composition have not been reported until now.

In this paper, we present neutron diffraction data for Cr–1.5% Fe and Cr–2% Fe alloy single crystals and report that neither the AF_1–AF_0 transition nor the transverse–longitudinal spin flip transition were observed for the Cr–1.5% Fe alloy. Using the experimental data of the 1.5% Fe specimen, we determined the phase boundary more accurately. We also report that no re-entrant ISDW phase exists for the magnetic phase diagram of CrFe binary alloy.

2. Measurements

Neutron diffraction measurements were performed at the HQR (T_{1-1}) triple-axis spectrometer installed at a thermal guide of JRR-3M, JAERI Tokai, Japan. The incident neutron energy was 13.9 meV. To minimize the $\lambda/2$ component of incident neutrons, a thick graphite filter was set between the monochromator and the sample table. Samples were Cr–1.5% Fe and Cr–2% Fe single crystals, which were once used to investigate a strain wave (second harmonics of the SDW) by x-ray diffraction [4] and have volumes of about 0.02 cm^3 and 0.005 cm^3, respectively. Magnetic scattering was studied around the 001 reciprocal lattice point on the $(1\bar{1}0)$ scattering plane. In this alignment, there are no satellite reflections on the axis in the vertical direction that passes through the 001 reciprocal lattice point for multi-domain specimens. Therefore, even though the instrumental resolution for the vertical direction to the scattering plane is rather poor, no contribution from any satellite position is observed at 001. Thus, any magnetic peak observed at the 001 reciprocal lattice point is ascribed to the commensurate antiferromagnetic state in this setting. Data were taken in the temperature range between 9 K and 300 K by using a refrigerator unit.

3. Experimental data and analysis

All experimental data were taken around the 001 reciprocal lattice point on the $(1\bar{1}0)$ scattering plane by scanning along the scattering vector ($\theta - 2\theta$ scan). Typical diffraction patterns for the Cr–1.5% Fe specimen are given in figure 1. The diffraction pattern has a weak peak at 001 in addition to the well defined satellite reflections observed around $001 \pm \delta$ ($\delta = 0.035$). Since the $\lambda/2$ component of the 200 nuclear Bragg reflection was almost completely (less than 10^{-6}) eliminated, the weak peak at 001 is considered to be magnetic in origin. The temperature dependences of the satellite peak and the 001 magnetic peak intensities are plotted in figure 2 on different scales. The satellite peak disappears at around 275 K, which corresponds to the T_N of the Cr–1.5% Fe alloy. The 001 peak, however, disappears at a temperature lower than T_N by about 30 K. The 001 peak intensity shows an anomaly at around 210 K. We will discuss these points later in more detail.

The main magnetic contribution of this specimen is the satellite peaks observed around $001 \pm \delta$. The temperature variation of the satellite peak behaves like an order parameter and no anomaly is observed in the whole temperature range. If the AF_1–AF_0 transition or the spin flip transition from the transverse SDW (TSDW) to the longitudinal SDW (LSDW) exists, the $001 \pm \delta$ satellite reflections should disappear below these transition temperatures. No such behaviour is observed. Thus, we can conclude that the Cr–1.5% Fe alloy shows the SDW state in the whole temperature range below T_N.

Now, let us consider the weak peak observed at 001. Usually an alloy specimen has an inevitable inhomogeneous distribution of solute atoms. Since the Cr–1.5% Fe alloy is located rather close to the AF_1–AF_0 phase boundary, a small fraction of the specimen with higher Fe concentration than the phase boundary shows the AF_1–AF_0 phase transition and yields a magnetic peak at 001. From the intensity ratio of the 001 reflection to the satellite peak, the volume fraction showing the AF_1–AF_0 phase transition is estimated to be 1.7% of the total volume under the assumption of an equal distribution of magnetic domains. This is not an unreasonable value for concentration fluctuations of this alloy. Thus, the temperature variation of this 001 magnetic peak gives us interesting information as to the phase boundary of this system.

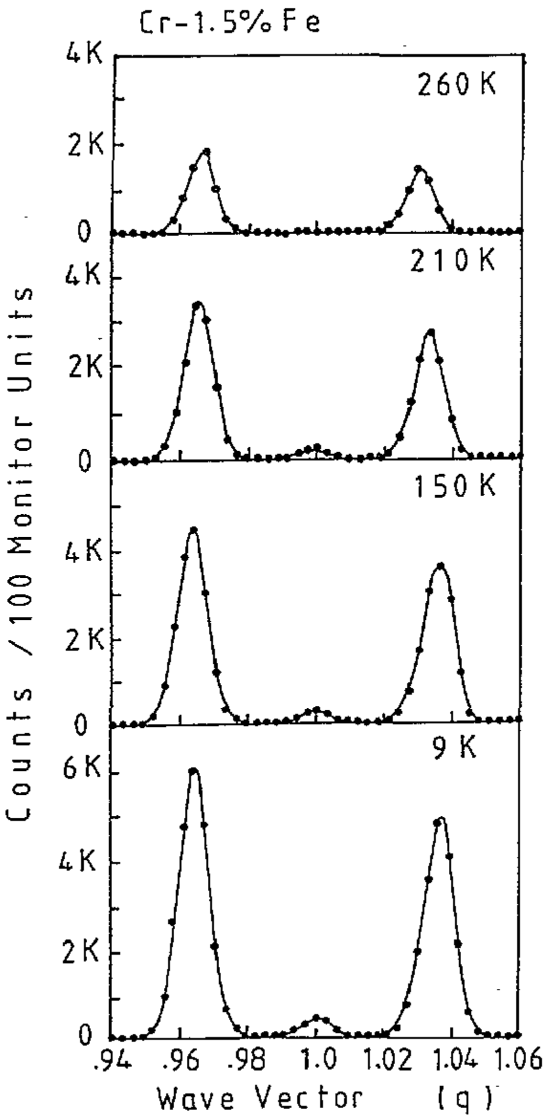

Figure 1. Diffraction patterns of satellite reflections for the Cr–1.5% Fe alloy observed by scanning along the scattering vector. See the text for a discussion of the weak central peak.

(i) The 001 magnetic peak completely disappears around 250 K. This temperature is considered to be the tricritical point and is consistent with the phase diagram previously reported (see figure 4).

(ii) Although the temperature variation of the 001 magnetic peak intensity has a slope near the transition temperature, probably due to the distribution of Fe concentration, the existence of a turning point of the slope (~ 210 K) indicates that the AF_1–AF_0 phase transition is of first order, consistent with the previous data [4–7].

(iii) Below the turning point, the 001 peak intensity increases monotonically with decreasing temperature. This indicates that there is no re-entrant incommensurate phase

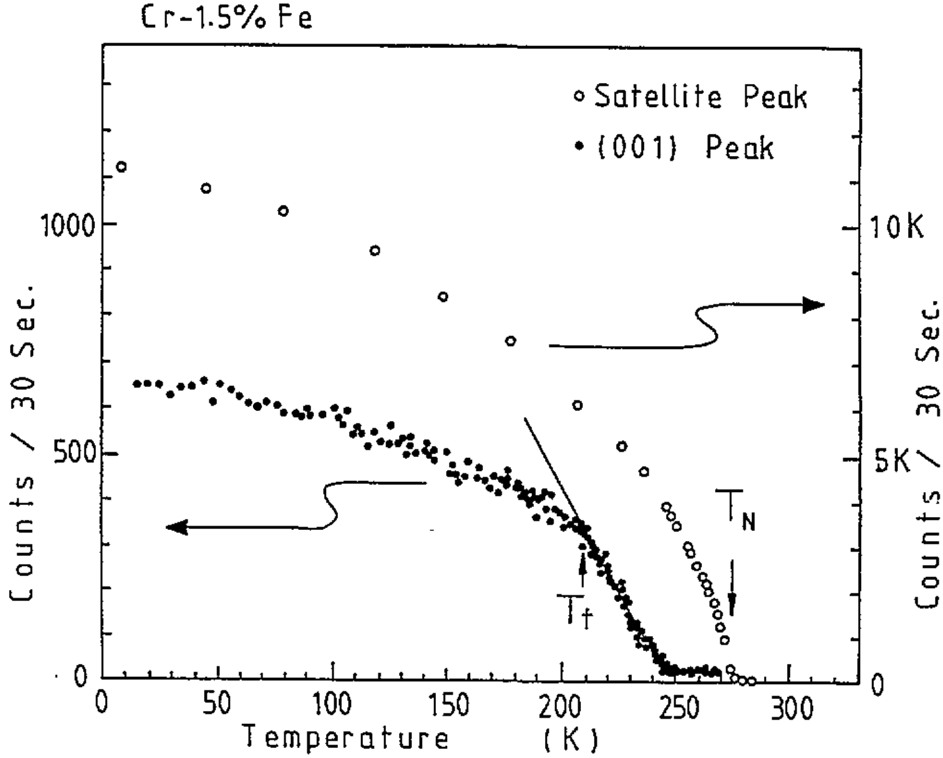

Figure 2. The temperature variations of the satellite peak and commensurate peak intensities.

as recently reported for the CrFeMn ternary alloy system [3], otherwise the commensurate peak intensity would decrease below the re-entrant transition temperature. This also suggests that the AF_1–AF_0 phase boundary is almost vertical.

Diffraction patterns observed for the Cr–2% Fe sample at several different temperatures are given in figure 3. Coexistence of the satellite reflections and the 001 reflection is again ascribed to the inhomogeneous distribution of Fe concentration. Note the temperature dependence of the satellite peak positions. The distance from the 001 reciprocal lattice point, δ, decreases with decreasing temperature in contrast to other ISDW states in Cr and Cr alloys. This is consistent with previous x-ray diffraction data [4] and explains the fact that the commensurate antiferromagnetic phase (AF_0) is located at a lower temperature than the ISDW phase (AF_1).

4. Discussion

The Cr–1.5% Fe alloy undergoes neither the AF_1–AF_0 phase transition nor the spin flip transition from the TSDW to LSDW phases and shows the TSDW state in the whole temperature range below the Néel temperature. The small anomaly reported by Butylenko [6] in his thermal expansion data of the alloy with the same Fe concentration (line 6 of figure 1 in [6]) could be ascribed to the AF_1–AF_0 transition of a small fraction in his specimen. This is due to the inhomogeneity of the Fe concentration in his specimen just as in our case.

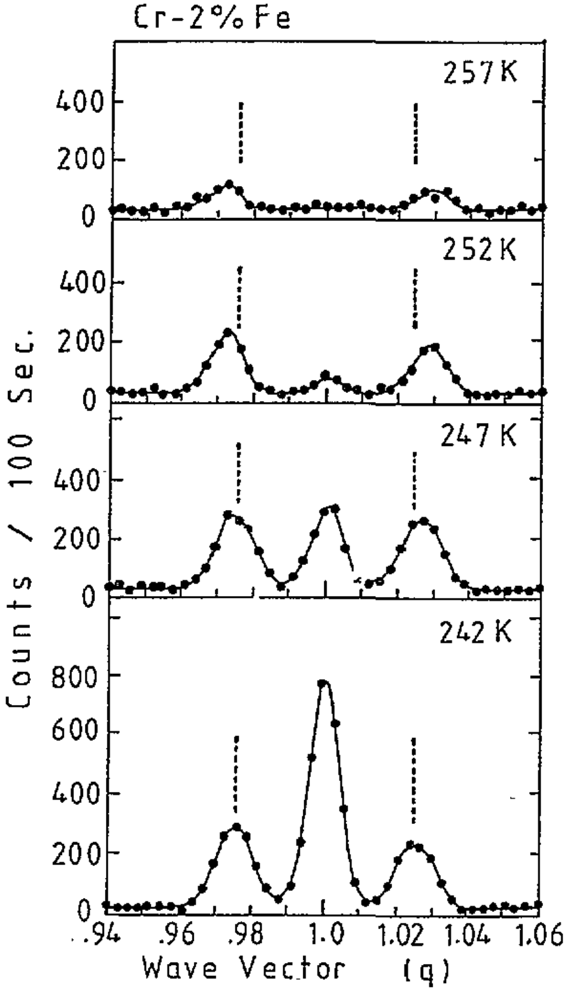

Figure 3. Diffraction patterns of the Cr–2% Fe alloy observed around 001 by scanning along the scattering vector. The broken lines indicate the satellite peak positions at $T = 242$ K.

Fawcett and Galkin recently observed [3] a phase change from the commensurate antiferromagnetic phase to the ISDW phase with decreasing temperature in CrFeMn ternary alloys. Since the ISDW phase is located at a higher temperature than the commensurate phase near the Néel temperature for this system, the lowest phase was named as a re-entrant incommensurate phase. Thus, one of the interesting points in the phase diagram of the CrFe binary alloy is whether the re-entrant incommensurate phase exists or not. The present magnetic scattering data observed at the commensurate peak position did not show any indication of the re-entrant incommensurate transition. They rather show that the phase boundary is almost vertical, because the temperature variations of both commensurate and satellite peak intensities behave like normal order parameters. The temperature dependence of the magnetic domain distribution may have some influence on the magnetic scattering intensity at the 001 position. The scattering line profiles shown in figure 1 were studied many times at low temperature for investigation of the magnons in this sample [8]. The

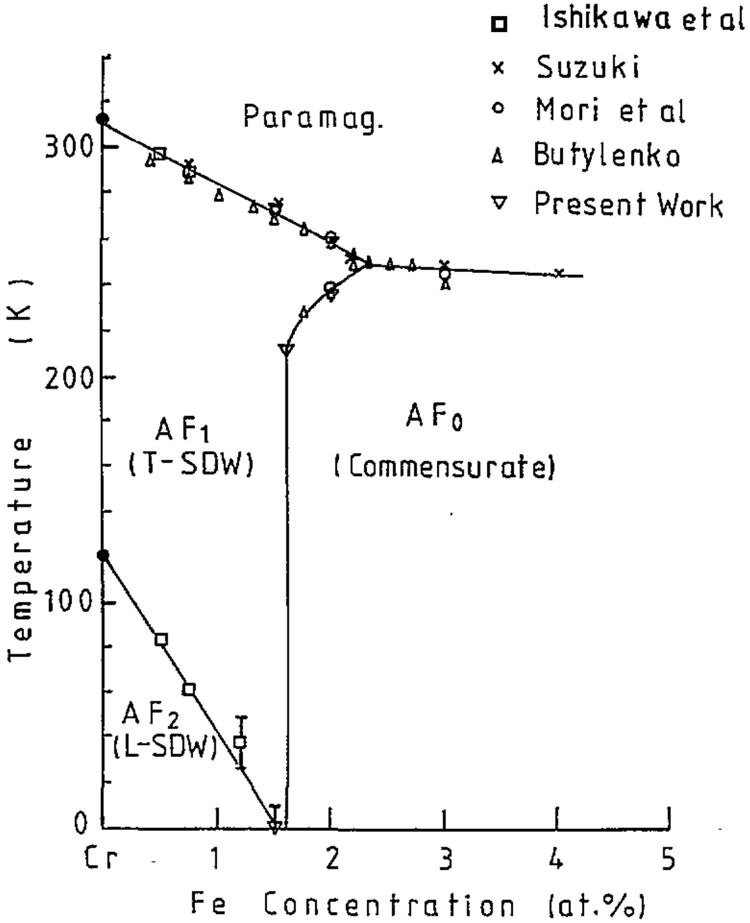

Figure 4. The phase diagram determined from the data published by previous authors and the present data.

001 peak intensity is reproducible after many cooling cycles, indicating that the domain structure of this specimen is stable with respect to thermal cycling.

Let us try to determine the AF_1–AF_0 phase boundary more precisely. Since the volume fraction showing the commensurate peak is very small (~ 1.7%) for the Cr–1.5% Fe alloy specimen, the phase boundary is not very close to 1.5% Fe. On the other hand, the thermal expansion anomaly studied by Butylenko [6] is distinctive for the specimen with 1.75% Fe, indicating that most of the volume fraction undergoes the AF_1–AF_0 transition for that specimen. We can say again that the phase boundary is not very close to 1.75% Fe. *Thus, the phase boundary is located at Fe concentrations between 1.5% and 1.75% and is not* very close to either of them. Since the phase boundary is considered to be almost vertical, the key point is the Fe concentration at the turning point of the slope in the temperature variation of the commensurate peak intensity. The transition temperature reported for the 1.75% Fe alloy is higher than the temperature of the turning point by about 15 K. From the extrapolation of the phase boundary curve, the turning point is estimated to be 1.62 (±0.03)% Fe.

The phase diagram using the data of previous authors [4–7] and the present data is given in figure 4.

5. Conclusions

The commensurate–incommensurate SDW phase boundary of CrFe alloys has been determined accurately using neutron diffraction of single crystals. The phase boundary is located at around 1.62(±0.03)% Fe and almost vertical with Fe concentration. The re-entrant ISDW phase does not exist in the magnetic phase diagram of CrFe binary alloys.

References

[1] See the references in Fawcett E 1988 *Rev. Mod. Phys.* **60** 209
Fawcett E *et al* 1994 *Rev. Mod. Phys.* **66** 25
[2] Friedel J and Hedman L E 1978 *J. Physique* **39** 1225
[3] Fawcett E and Galkin V Yu 1992 *J. Magn. Magn. Mater.* **109** L139
[4] Mori M, Tsunoda Y and Kunitomi N 1976 *Solid State Commun.* **18** 1103
[5] Ishikawa Y, Hoshino S and Endoh Y 1967 *J. Phys. Soc. Japan* **22** 1221
[6] Butylenko A K 1989 *Phys. Met. Metallogr.* **68** 37
[7] Suzuki T 1976 *J. Phys. Soc. Japan* **41** 1187
[8] Tsunoda Y and Nicklow R M *Int. Conf. Neutron Scattering '94 (Sendai)* submitted