Noncommensurate atomic structure of the alloy Ni+67.7 at.% Fe

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A neutron-diffraction method was used to investigate an iron-nickel single crystal with 67.7 at.% Fe. The neutron-diffraction pattern at room temperature has revealed, for the first time, superstructure reflections that are regularly arranged in the reciprocal lattice. The scattering patterns are easiest to interpret within the framework of an atomic structure that is noncommensurate with the principal fcc lattice.

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In recent studies[1,2] it has been shown, by x-ray diffraction and electron-diffraction methods, that some latent changes of the atomic structure of the alloys takes place in the initial fcc phase long before the martensitic transition. This has served as a further stimulus for an extensive discussion of the details of the fcc $\rightleftharpoons$ bcc transition and its connection with the Invar properties of alloys. Interest attaches therefore to a neutron-diffraction investigation of the atomic fine structure of disordered single-crystal samples of Invar Fe-Ni alloys.

In the present study we investigate a single crystal containing a 67.7 at.% Fe. The sample was a sphere of 12 mm diameter. The wavelength λ of the neutrons obtained by reflection from a double monochromator (we used in this experiment a pair consisting of copper and lead crystals) was 1.4 Å. The admixture of neutrons with $\lambda/2$ was approximately 1%.

The investigated thin crystals had an axis orientation [100] $\perp$ q (q is the scattering vector). The neutron scattering intensity was measured in the intervals

$$0 < \sin\theta/\lambda \sim |\mathbf{q}| < 0.35 \text{ and } 0 \leqslant \psi < 360°,$$

(2θ is the angle between the wave vectors of the incident and scattered waves; ψ is the angle between the [100] direction in the scattering plane and q).

The neutron-diffraction patterns of the disordered alloy Ni+67.7 at.% Fe, obtained at room temperature, has revealed a large number of coherent superstructure reflections. Figure 1 shows some of the strongest peaks: in the upper part of the figure as a function of the angle ψ (at fixed θ), and in the lower part as a function of $\sin\theta/\lambda$ (at fixed ψ). For an estimate of the intensity of the observed reflections, Fig. 1 shows also the reflection $(220)\lambda/2$.

The total distribution of the observed intensity is conveniently represented in reciprocal space. The circles in Fig. 2 show the positions of the reflections in the reciprocal lattice. The diameter of the circle corresponds to the angular

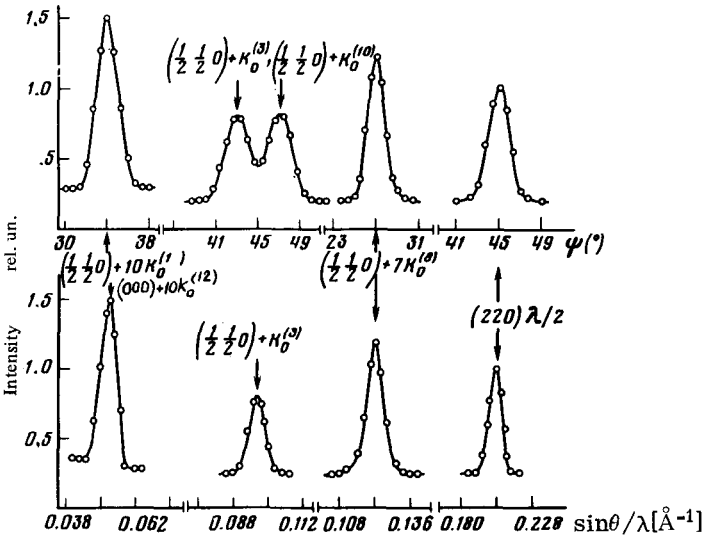

FIG. 1. Strong superstructure reflections (satellites) in comparison with the intensity of the (200) peak.

dimension of the peak at half its height. The observed pattern of the reflections is symmetrical about the [100] direction, and the figure shows therefore only the upper part of the reciprocal lattice relative to the (000) site. Depending on the intensity, the superstructure reflections in Fig. 2 are divided approximately into three groups. The intensity of the peaks with the thick contours is not less than the intensity of $-(220)\lambda/2$. The thin contour marks reflexes whose intensity is approximately one third of $-(220)\lambda/2$. The dashed contours denote reflections weaker than the $(220)\lambda/2$ intensity by approximately one order of magnitude.

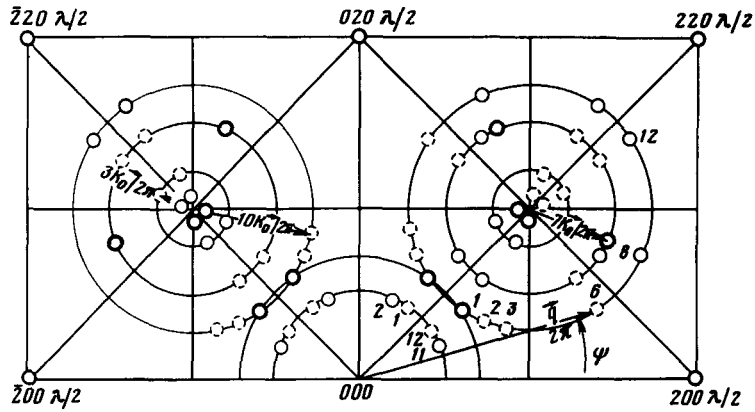

FIG. 2. Position of satellites in the reciprocal lattice.

The spatial distribution of the reflections in the reciprocal lattice is most symmetrical about the (000) site and the positions $\frac{1}{2}\ \frac{1}{2}\ 0$ and $\bar{\frac{1}{2}}\ \frac{1}{2}\ 0$. A similar distribution is observed in the vicinity of the multiple positions of the type $\frac{1}{2}\ \frac{3}{2}\ 0$ and $\frac{3}{2}\ \frac{3}{2}\ 0$, but owing to the lower intensity and the poorer resolutions at large scattering angles, the exact location of the superstructure reflections in the reciprocal lattice is difficult and is not shown in Fig. 2.

Outwardly the scattering picture corresponds to a magnetic structure with a large superperiod, of the type of a complex helix. It is difficult to assume, however, that these alloys contain antiferromagnetic interactions strong enough to make such a structure stable up to several hundred degrees.

The origin of the superstructure (satellites) is easiest to understand by assuming a regular character of the displacements of the atoms in the fcc lattice, for example sinusoidal.[3] It is shown in[3] that similar scattering pictures are observed in experiment in a number of compounds near diffusionless phase transitions, and the satellites in the reciprocal lattice are disposed at a certain distance $n\mathbf{k}_0/2\pi$ ($n\mathbf{k}_0$ is a wave vector on the order of n) from the sites corresponding to the usual, doubled, tripled, etc. chemical unit cell of the "parent phase." A characteristic attribute of the model of the atomic displacements in the crystal (modulation of the scattering phase) is the presence of higher "diffraction harmonics" $n\mathbf{k}_0$. These structures have been dubbed noncommensurate atomic structures (in analogy with magnetic helicoidal structures).

In our case, the satellites in Fig. 2 are disposed, relative to the sites of the doubled cell, at distances that are multiples of $|\mathbf{k}_0|/2\pi$ along strictly defined directions in the lattice. In the reciprocal-lattice plane (001) we can distinguish twelve such directions, which are apparently connected with the presence of twelve specific displacement domains in the alloy. They are arbitrarily numbered counter-clockwise in Fig. 2. The directions 1, 2, 3 relative to the site ($\frac{1}{2}\ \frac{1}{2}\ 0$) divide the angle 45° into four equal parts, while the remaining directions (j) are connected with them by a fourfold symmetry axis. The observed diffraction pattern depends essentially on the composition and on the temperature. These results will be published in greater detail later on.

Thus, a neutron-diffraction investigation shows that near the martensitic transformation 1) an intermediate atomic structure is realized in the alloy Ni + 67.7 at.% Fe and is noncommensurate with the principal fcc lattice. Further study of its singularities will apparently uncover some important details of the involved problem.

[1)]In iron-nickel alloys, precipitation of the martensite at room temperature begins with 70 at.% Fe.

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