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X-ray Diffraction Data for the Study of the Multilevel Nanostructures in Ni_3Fe Deformed Single Crystals

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Abstract

X-ray analysis has been applied for the study of the formation of nanostructures as the result of plastic deformation in Ni_3Fe single crystals with the $L1_2$ structure. It was shown that the main structural changes in ordered alloys had the features similar to pure metals and the disordered solid solutions but were more complex. Structure consists of nano-crystallites divided by the antiphase boundaries forming the elements having the size a ten times smaller than the dimensions of the crystallites. After the strain of 0.18 together with the antiphase domains with the average size equal to 14 nm a small fraction of domains with an average size of 10-11 nm was revealed. After the strain of 0.38 or more, the average size of the antiphase domains was reduced to 5-2 nm.

Keywords: X-ray analysis, ordered alloys, Ni_3Fe, $L1_2$ structure, antiphase boundaries, nano-crystallites

1. Introduction

The nanostructured materials created by the different ways are of the special interest since the presence of nanoscale components in structure leads to appearance of new functional properties. The perspectives in this sense have the alloys with the long-range atomic order [1-9]. In the ordered alloys the superdislocations [10] are able to generate in its motion the specific planar defects – antiphase boundaries. These structure defects substantially change the properties of the ordered alloys [11, 12]. The best research techniques of similar states are the diffraction methods, one of which is the method of X-ray diffractometry. In the present work the methods of X-ray diffraction

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analysis have been used for the study of the multilevel nanostructures formation after deformation in Ni_3Fe single crystals with the $L1_2$ structure at high degree of a long-range order.

2. Experimental procedure

Single crystals of the Ni_3Fe alloy were grown by the Bridgeman method in an argon atmosphere from Ni and Fe with degrees of purity of 99.99%. The ordered state was obtained by stepwise annealing of specimens at temperatures in the interval 550–300°C with a cooling rate of 5°C per day. Changes in the long-range order were studied for single-crystal plates 0.2 mm thick cut along the (100) plane. The specimens were cold-rolled (at 293 K) to provide different degrees of deformation (compression). The alloy state was studied by X-ray diffraction analysis. X-ray patterns were taken at room temperature using DRON-3 and DRON-1.5 difractometers with monochromatic FeK_α and CuK_α radiation. The long-range order parameter was determined in the usual way from the ratio of the measured integrated intensities of the (100) superstructural and the (200) fundamental lines with allowance for the required factors such as the multiplicity factor P, angular factor Φ and structure factor F [13]:

$$\eta^2 = I_{ss}(P\Phi F^2)_f \,/\, I_f(P\Phi F^2)_{ss}.$$

The domain sizes were determined from the integral width of the (100) line using the approximation by the Selyakov–Sherrer formula [13]. The microdistortions and sizes of coherent scattering regions were calculated using the procedure described in [14].

3. Results and discussion

The initial ordered state in Ni_3Fe single crystals had been reached by annealing for 1200 hours. The $L1_2$ crystal structure had been formed with the high degree of the long-range order. The measured long-range order parameter η_{eff} was equal to 0,98±0,02. The initial atomic structure consisted of the antiphase domains with the average domain size of (14±2) nm. The microdistortions Δd/d of the crystal lattice were close to zero and did not exceed 0.2 ± 10^{-3} value. Coherent scattering regions had the average size ⟨L⟩ more than one micron. Plastic deformation by rolling changed the state of the long-range order, reduced sizes of antiphase domains, decreased coherent scattering regions, and increased microdistortions of the crystal lattice (Fig. 1, 2).

The main change in the defect structure occurred at the initial stages of deformation before 0.18-0.2. There had been the intensive increase of microdistortions in crystal lattice (see Fig. 1.a) and the decrease of the average size of coherent scattering regions ⟨L⟩ up to 200 nm (Fig. 1.b).

After the degree of strain 0.18-0.2 the defects storage in crystal lattice leaded to the further growth of microdistortions (Fig. 1.a), but the rate of this growth with the increasing of deformation slowed down and the value of microdistortions varied slightly.

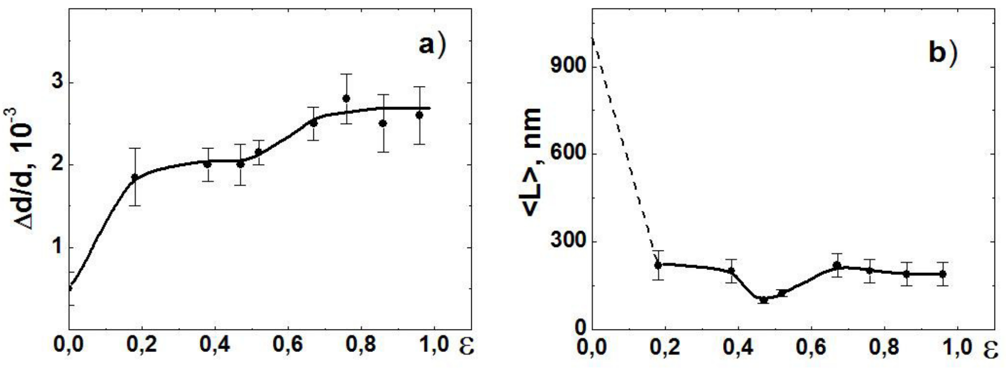

Fig. 1.Dependences of the microdistortions Δd/d (a) and the average size of coherent scattering regions ⟨L⟩ (*b*) on the degree of strain in Ni_3Fe (by rolling)