Disturbance of long-range order and single crystal state under plastic deformation in Ni_3Fe

Svetlana Starenchenko, Vladimir Starenchenko and Irina Radchenko
Tomsk State University of Architecture and Building, 2, Solyanaya sq., Tomsk, 634003, RUSSIA
email: star@tsuab.ru

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Abstract. In this paper the influence of plastic deformation on the long range order in single crystal Ni_3Fe is presented. A study of states of the thin and thick plates was performed by the X-ray methods. Heterogeneity of the structure is marked at deepening inside the material. It is established that plastic deformation causes disturbance of a single crystal state of the alloy and order-disorder phase transition. The lowering of the long-range degree of the alloy is accompanied by inhomogeneous decrease in the antiphase domains sizes. Heterogeneity of the order - disorder transformation is connected with the strain localization.

Introduction

Influence of plastic deformation on the long-range order has been investigated at milling the ordered alloys in ball mills [1-3]. Characteristics of the ordered alloys with different superstructures, after deformation by cold rolling, have been studied in our papers [4-6]. Researches were carried out on the alloys with superstructures $L1_2$, $L1_2$ (M), $L1_2$ (MM), $D1_a$. The basic features of the order – disorder phase transition induced by the plastic deformation were revealed. It has been established that the long-range order parameter decreases during deformation of alloys. Alongside with the ordered phase, there are areas of the disordered phase. The process of the long-range order disturbance is accompanied by inhomogeneous decreasing the antiphase domains sizes. There is a nonmonotonic change in values of areas of coherent scattering. The mentioned experimental researches were carried out for polycrystalline materials. The long-range order at the deformation of a single crystal was not studied, though there are a great number of papers in which results of studying deformation processes in single crystals have been presented. The present work investigates the effect of plastic deformation on the long-range order depending on the thickness of a sample. The long-range order parameters, the sizes of antiphase domains, and microdistortion have been measured by the x-ray methods

Experimental

A single crystal of the Ni_3Fe alloy was grown by the Bridgeman method under an argon atmosphere from Ni and Fe with degrees of purity of 99.99%. The ordered state was obtained by stepwise annealing of the specimens at temperatures in the interval 550–300°C with a cooling rate of 5°C per day. The ordering anneal was performed in quartz tube under argon. The samples were quenched to room temperature.

Changes in the long-range order were studied for single-crystal plates 2.5 mm and 0.2 mm thick. They were cut along the (100) plane. The samples were cold-rolled (at 293 K) to provide different degrees of deformation. The alloy states were studied by X-ray diffraction analysis. X-ray patterns were taken at room temperature using DRON-3 diffractometer 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 I_{ss} and the (200) fundamental I_f lines with allowance for the required factors such as the multiplicity factor P, angular factor Φ and structure factor F:

$$\eta^2 = I_{ss}(P\Phi F^2)_f / I_f(P\Phi F^2)_{ss}. \quad (1)$$

The microstresses in the material, domain sizes, and sizes of coherent scattering areas were calculated using the procedure described in [7].

Results and discussion

The superstructure $L1_2$ with high degree of the long-range order close to a one ($\eta \approx 0.98\pm0.02$) was detected in the initial state of single crystals of the alloy, which was ordered by heat treatment. The average antiphase domain size was equal to (14 ± 2) nm. The strains of the crystal lattice were close to zero.

The thin plate. To find out the effect of the plastic deformation on the long-range order of the single crystal Ni_3Fe, the plate 0.2 mm thick was rolled to different degrees of the strain.
Fragmentation of the deformable single crystal. Essential structure changes in the alloy Ni_3Fe have been revealed as a result of the deformation. First of all, the fragmentation of the single crystal was observed when the deformation attained $\varepsilon \approx 0.18$–0.2. On the specimen surface, that coincided with the (001) plane, disorientated microareas were observed and the fragmentation of the single-crystal was actualized. After $\varepsilon \approx 0.18$, the single-crystal state was disturbed. Fragments of the planes (113), (111) appeared additionally on the specimen surface. The higher the strain was the higher fraction of (113), (111) areas emerged in the process of deformation. At higher degrees of deformation, the fraction of the areas focused by planes (113) and (111) along the surface, increases. However, at all degrees of deformation, the fraction of the first areas is higher, and after $\varepsilon = 0.76$ it is much higher, than that of the second ones. Small intensity of reflection (022) comes into existence in the diffraction pattern of the sample deformed to $\varepsilon = 0.52$ and more. It testifies to the emergence of planes (011).

After plastic deformation $\varepsilon = 0.86$ of the single crystal Ni_3Fe with 0.2 mm thick, the fragmentation is such that the surface is occupied with planes (001) and (113) in equal quantity. The planes (111) and (011) occupy a

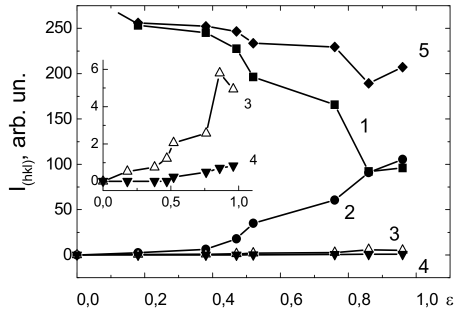

Figure 1. Dependences of intensities of X-ray reflections on the degree of strain in the Ni_3Fe alloy: 1 - I(002); 2- I(113); 3 - I(111); 4 - I(022); and) 5 - the sum of the intensities of all observed reflections ΣI(hkl)

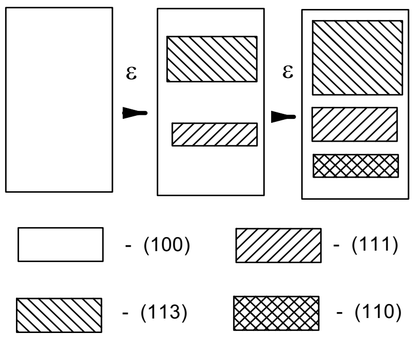

Figure 2. Schematic pattern of the fragmentation of the surface withincrease in the degree of strain in the Ni_3Fe alloy

small part on the sample surface as well. Dependences of the reflection intensities $I_{(hkl)}$ and the sum of the intensities of all observed reflections $\Sigma I_{(hkl)}$ are shown in Fig. 1. Intensity of the diffraction scattering in undeformed specimen is higher than that of the diffraction scattering in the deformed specimen. It can be explained by the fact that because of disorientation, separate sites of planes leave reflecting position. Also, it is possible to assume that some part of the material undergoes amorphization and creates diffuse scattering. The decrease in the intensity of both the superstructure reflections and the basic ones after milling of the alloy Ni_3Al in a ball mill has been observed in the

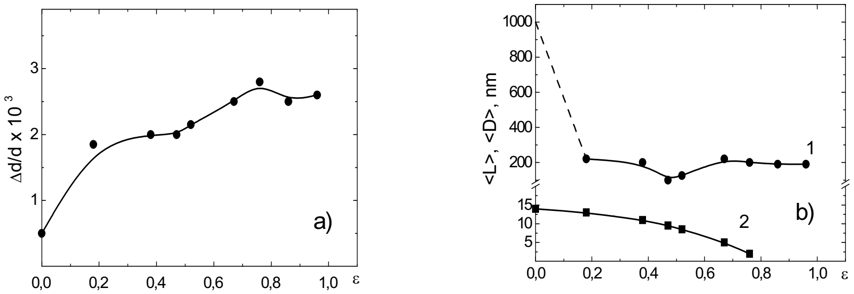

Figure 3. Dependence: a - microdistortions; b - average size of the crystallites (1), average size of the antiphase domains (2) on the degree of strain in the Ni_3Fe alloy

paper [3]. Emergence of many fragments focused by the reflecting plane (113) on surface of the sample at the first stages is caused by the fact that the angle between planes (001) and (113) is the least. The minimum angles between planes (001) and (113), (111), (110) are equal to 25°14′, 54°44′ and 45°, and between (113) and (111), (110) - 29°30′ and 31°29′ respectively. Occurrence of the areas focused by planes (111) parallel to the surface can be explained by a small angle between (113) and (111). Only high degrees of deformation create the fragments focused by planes (110) parallel to the surface (Fig. 2).

Deformation influence on sizes of crystallites, antiphase domains, and value of strain of crystal lattice. Accumulation of deformation defects leads to an increase in microdistortions of the crystal lattice (Fig. 3.a). Increase in Δd/d is more intensive when the strain is raised to $\varepsilon \approx 0.18$–0.2. Then the increasing of Δd/d is moderated, and the microdistortions change nonmonotonically after $\varepsilon \approx 0.52$ with a further increase in strain, because relaxation processes occurring during deformation result in the formation of a dislocation substructure. Disorientation of microareas leads to the appearance of crystallites and their average size decreases during deformation (Fig. 3.b.1). Average size of the antiphase domains decreases as well (Fig. 3.b.2). Decrease in the antiphase domains sizes is inhomogeneous. Thus, initial single-crystal specimens undergo fragmentation during deformation process. The average size of the crystallites becomes noticeably smaller at plastic deformation. The greatest decreasing is observed before $\varepsilon \approx 0.18$. After $\varepsilon \approx 0.46$ when the average size of the crystallites attains its minimum, some increasing of coherent regions occurs. The reason is that reorganization of the dislocation structure is realized. The changes in average size of the antiphase domains accompany

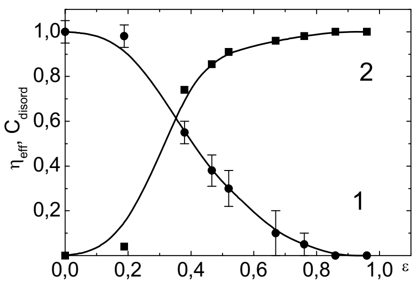

Figure 4. Dependence: 1 - effective long-range order parameter; 2 - volume fraction of disordered phase on the degree of strain in the Ni_3Fe alloy

plastic deformation. Sizes of antiphase domains get smaller during deformation. (Fig. 3.b).

Influence of plastic deformation on the long-range order. Plastic deformation induces processes of disturbance of the long-range order. This is confirmed by the decrease in the intensity of the superstructure reflection (001) as compared to the intensity of the fundamental reflection (002) and hence, in the long-range order parameter. (Fig. 4.1). Strain $\varepsilon \approx 0.18$ causes a slight decrease in the long-range order parameter. The intensity of the superstructure reflection (001) drastically reduces after $\varepsilon \approx 0.2$ and continues to decrease at further deformation. The superstructure reflection (001) is spread very much after $\varepsilon \approx 0.67$. Due to this, the diffraction superstructure reflection could hardly be separated from the background. It can be said with confidence that the Ni_3Fe alloy becomes disordered after $\varepsilon \approx 0.86$.

It has been noted [6], that the mechanisms, causing deformation-induced order-disorder transition, determine heterogeneous character of the latter. It is possible to believe, that decrease in the value η_{eff} takes place due to occurrence of the disordered defective phase. It is difficult directly to observe attributes of the two-phase state because of the small distinction of parameters of the lattice of ordered and disordered phases in alloy Ni_3Fe ($\Delta a=(a_{dis}-a_{ord})=0,0003$ nm) [8], and because of the reflections broadening caused by the presence of deformation defects. Fractions of ordered C_{ord} and disordered C_{disord} phases can be calculated, taking into account that

$$\eta^2_{eff}=C_{ord}\,\eta^2_{ord}, \tag{2}$$

and

$$C_{disord}=1 - C_{ord}. \tag{3}$$

The dependence of the volume fraction of the disordered phase C_{disord} on the degree of strain in the Ni_3Fe alloy (Fig. 4.2) has been calculated in the assumption that in local places of the ordered phase which have been not covered by deformation processes $\eta_{ord}=1$. The most intensive decrease in the effective long-range order parameter occurs in the interval of deformations $\varepsilon=0.2\div0.46$. The long-range order remains constant at the first stage of deformation, and appreciable decrease in the degree of the long-range order begins only after $\varepsilon=0.2$. The rate of decreasing η_{eff} is maximum at $\varepsilon=0.38$, further decreasing occurs more slowly. The decrease in the value of the long-range order parameter is more noticeable in polycrystalline alloys [4-6] at identical strains and close values of the ordering energy, like in the Ni_3Fe alloy. The reason is that decrease in the degree of the long-range order occurs after certain accumulation of defects of different types in the material, and boundaries of grains is the essential defect of a crystal lattice stimulating intensive disturbance of the long-range order.

The thick plate. The study of the thick plate deformation after cold rolling showed complexity of this process. Structure states on the surface differed from those within the material. The sample was a single crystal, and its surface coincided with the plane (001) up to the deformation degree ε = 0.15 – 0.17.

Fragmentation of the deformed single crystal. The crystallographic disorientation of microareas of the crystal occurred after the deformation degree ε = 0.15 – 0.17, and the planes (111) and (113) emerged in reflecting positions. Besides reflections (002) and (001), reflections (113) and (111) were fixed in diffraction patterns at ε=0.17 and ε=0.19 as well. Intensities of reflections of both types were practically identical but they were much lower than the intensity of reflections from the plane (001). The fraction of planes (113) exceeded the fraction of planes (111) at the deformation ε=0.19. Weak reflections (022) were also observed at both deformations. Lines (111), (113), (022) were considerably broadened and were asymmetrical due to the disorientation of surface and undersurface layers. It is possible to assume that a part of the planes occupies a slightly incorrect reflecting position and due to the bend of the lattice is deflected at a small angle.

The state inside the material differs from the state on the surface. It has been found out that after skimming the layers of different thickness in the material, the fraction of the areas occupied with

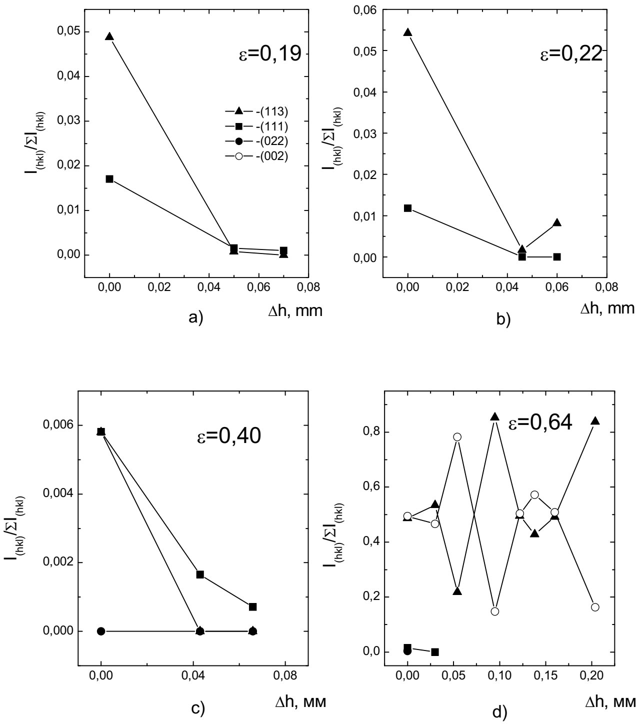

Figure 5. Dependences of relative intensities of the reflection on the distance from the surface of the Ni_3Fe alloy: a – $I_{(113)} / \Sigma I_{(hkl)}$; b – $I_{(111)} / \Sigma I_{(hkl)}$; c – $I_{(022)} / \Sigma I_{(hkl)}$; d – $I_{(002)} / \Sigma I_{(hkl)}$, *where* $\Sigma I_{(hkl)} = I_{(113)} + I_{(111)} + I_{(022)} + I_{(002)}$

planes (113) decreases faster than the fraction of planes (111). Reflecting planes (113) are absent at a depth of Δh = 0,04 mm, and the reflecting surface is the only plane (001) with a small fraction of the fragments focused parallel to the surface by the plane (111) at a depth of Δh = 0,07 mm (Fig. 5. a and b).

In a similar manner, the fragmentation takes place at higher degrees of deformation (Fig. 5. c). It should be noted that the deformation process which occurs at cold rolling of the single crystal Ni_3Fe, is spread to a depth of ~0,12 mm at ε=0,47. Basically, the planes (113) appear on the surface (001) of the sample at ε=0.56. This fraction exceeds the fraction of the surface occupied with planes (111); there is also insignificant quantity of fragments of planes (110). Heterogeneity of the structure is marked at deepening inside the material. Actually, the fragmentation decreases in undersurface layers, as well as at lower degrees of deformation. The material is a single crystal at a depth of ~0.1 mm but reflecting planes are distorted. Deformation process completely covers the sample ~0.6 mm thick at ε increasing up to 0.64 (Fig. 5. d).

However, the fragmentation areas of the material are placed inhomogeneously inside the sample at various depths. Fragments of the material with reflecting planes (110) and (111) are concentrated mainly near to the surface. As to the areas with the planes (113), focused along the surface, they exist both on the surface and in the depth of the sample alongside with planes (001). The volume fraction of areas (113) changes nonmonotonely according to the sample thickness. Structural characteristics of the material change simultaneously with accumulation of the defects of the single crystal Ni_3Fe. The values of microdistortions, the average sizes of the crystallites, and the long-range order of the alloy change as well.

Microdistortions of the crystal lattice Δd/d decrease when depths of layers increase (Fig. 6. a). Sizes of coherent scattering regions inside the material are noticeably smaller than those on the surface of the specimen (Fig. 6. b).

This can be explained by the deformation inhomogeneity. Obviously, superficial layers are under the greatest influence, and internal layers are distorted to a lesser degree (Fig. 6. a). Perhaps, it is connected with the fact that the dislocation structure varies in different volumes of the sample. Inside the rolled plate, the dislocations are distributed uniformly and it corresponds to small sizes of the areas of coherent scattering. In the vicinity of the surface, the formation of the non-uniform distribution of dislocations occurred most likely (Fig. 6. b).

In this case, in the alloy there are faultless areas of large sizes, which are cleared of dislocations and are encircled with the material of high density of dislocations. The obtained results are reasonable. Investigation of the dislocation structure corresponding to different degrees of deformation revealed that small degrees of deformation create more homogeneous substructures. High deformations lead to non-uniform distribution of dislocations [9].

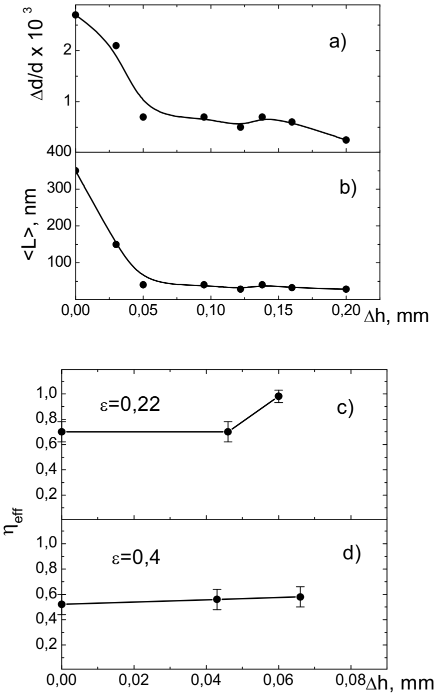

Figure 6. Dependence: a - microdistortions; b - average size of the crystallites; c - long-range order parameter (ε=0.22); d - long-range order parameter (ε=0.4) on the distance from the surface of the Ni_3Fe alloy

Influence of plastic deformation on the long-range order. Deformation also influences the states of the long-range order. In the range of strains ε=0÷0.12, the effective parameter of the long-range order η_{eff} does not change within the limits of the experimental error of measurements. Significant decrease in the long-range order parameter η_{eff} begins at deformation ε=0.14 and proceeds under further deformations ε=0.17, ε=0.2. It has been found out that both the long-range order and single crystal are kept inside the sample at the strain ε=0.19. The long-range order parameter η_{eff} is equal to 0.70 at ε=0.22, but its value is 0.98 at a depth of 0.06 mm (Fig. 6. c). When the sample was deformed to ε= 0.27, 0.32, 0.40, 0.47 the effective parameter of the long-range order remained appreciably below 1 (Fig. 6. d) after skimming the layers of the material from the surface up to the disappearance of fragmentation. Further deformation leads to spreading the disturbance of the long-range order, as well as to the disturbance of the single crystal to farther distance from the surface of the sample.

Thus, the disturbance of the long-range order at small deformations by cold rolling occurs mostly near facial layers where the density of deformation defects is higher. The change in the long-range order parameter can be unmonotonous with the depth because processes of deformation localization and the deformation inhomogeneity.

Conclusions

1. Plastic deformation of the single crystal Ni_3Fe disturbs the single crystal state of the alloy when storage of dislocations and their redistribution in the crystal cause the emergence of disorientated microareas.
2. The strain-induced order - disorder phase transition takes place in the ordered alloys. It happens when the significant quantity of defects of crystal lattice of different types (dislocations, point defects, deformation antiphase boundaries) is accumulated in local places of the strained alloy.
3. Drastic decrease in the long-range order in the Ni_3Fe alloy occurs when the disorientation of microareas and the fragmentation of the alloy begin.

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