Influence of crystals orientation on parameters of Ni$_3$Fe dislocation structure

L A Teplyakova$^1$, T C Kunitsyna$^2$ and N A Koneva$^1$

$^1$Tomsk State University of Architecture and Building, Physics Department, Tomsk, 634003, Russia
$^2$Tomsk State University of Architecture and Building, Higher Mathematic Department, Tomsk, 634003, Russia

E-mail: lat168@mail.ru

Abstract. At present the basic evolution laws of the dislocation structure forming in the differently oriented Ni$_3$Fe monocrystals under pressing were established. While the data about the dislocation structure quantitative parameters and their behaviour during deformation at different crystal orientations are missing. In the paper the correlation of the sequence of change of substructures forming in the Ni$_3$Fe monocrystals with the sequence of change of deformation stages has been revealed. The monocrystals with the deformation axis orientations [001], [111], [011] and [1.8.12] were studied. For the all mentioned deformation axis orientations the quantitative characteristics of dislocation structure were determined and their connection with the deformation curve parameters was revealed.

1. Introduction

It is known that at one axis loading the laws of formation of the dislocation structure and work hardening of the metal monocrystals and solid solutions depend significantly on their orientations [1-3]. In this case the Ni$_3$Fe alloy with a short range order is the most investigated one [4]. In the monocrystals with the deformation axis orientation corresponding the apexes (orientations [001], [111], [011], [1.8.12]) and the internal part (orientations [1.8.12]) of the stereographic triangular the inhomogeneous net substructure with the alternate layers with the decreased and increased dislocation density is formed. In [1.8.12] monocrystals one system of layers is observed [4, 5]. In [001], [111] and [011] monocrystals one can see two, three and four systems of layers according to numbers of equally loaded slip planes in each of them [4]. In spite of the fact that in the monocrystals with the deformation axis orientation [111] and [001] the number of equally loaded slip planes (acting within the whole volume) is higher than in [011] monocrystals, the number of locally acting planes, as a rule, is less than two [6]. Thus, during the plastic deformation the [011] monocrystal is separated into areas where the dislocation substructure evaluates as in the crystals oriented for a single slip, [001] monocrystal is devided into the areas where it develops as in [011] monocrystals and inside them, in its turn, as in the monocrystals with “mild” orientation. In the latter one sees the change of substructure types in the following succession: plane and quasi plane pile-ups and multipoles → plane and quasi plane nets → three dimensional dislocation net structure [4, 5]. The present paper is devoted to measurement of the quantitative characteristics of evaluating net substructure, construction of their
distributions and determination of the connection with the hardening curve parameters for the all investigated monocrystal orientations.

2. Materials and experimental procedure
In the paper the Ni$_3$Fe monocrystals with the short range order oriented for single (orientation [1.8.12]) and multiple slip (orientations [001], [011], [111]) were investigated. The monocrystal orientations were determined by the Laue method and epigrams. Deformation was carried out by pressing on the samples with the size of 3 x 3 x 6 mm$^2$. The deformation rate was equal to $1,5 \cdot 10^{-2}$с$^{-1}$.

3. Results and Discussion

3.1. Dependencies “τ – ε”
The deformation curves for different investigated orientations of the Ni$_3$Fe monocrystals in τ – ε coordinates (τ is the shift stress in the primary plane of octahedron slipping) are given in Figure 1. Here and next the following notations of the monocrystal deformation axis orientation are used: 1 – [001], 2 – [111], 3 – [011], and 4 – [1.8.12]. The Figure 1 shows that the monocrystal orientation essentially influences the character of hardening. The monocrystal deformation curves were analyzed by differencing the “τ – ε” dependences (dτ/dε = θ – the deformation hardening coefficient).

![Figure 1. Strain curves of single crystals of the alloy Ni$_3$Fe. Orientation axis deformation of crystals.](image)

Figure 2 shows the “d τ/d ε – ε” dependencies for the monocrystals of the investigated orientations. As it follows from Figure 1 and Figure 2 the staging is the most general property of all presented deformation curves. In the investigated monocrystals rather complex staging spectrum is observed. The analysis of the dependences given in Figure 2 testifies to the fact that in the monocrystals with the axis deformation orientations [001] and [111] as well as in the polycrystals [7] the deformation curve has four stages (the transitional stage with the increasing θ value, the stage II with the largest value of θ, the stage III where the θ value is decreasing and the stage IV with low and almost constant the θ value). In this case the orientation [001] appears after quite deep deformations.

The monocrystals [1.8.12] and [011] have slightly different type of staging. In the beginning of plastic deformation one observes the stage characterized by the constant value of θ. This stage cannot be classified as the true stage I because here the θ value is rather large (100÷200 MPa) [8]. It should be better named as the stage II$_1$. The stage II$_1$ is changed by the stage π which is transitional to the stage II$_2$ characterized by greater hardening coefficient as compared with that at the stage II$_1$. Finally in monocrystals [1.8.12] and [011] the stage II$_2$ turns gradually into the stage III. A clear idea about the θ behavior at different stages of the monocrystal deformation with the different deformation axis orientation may get from Figure 2. Thus the monocrystal deformation curves of the investigated alloys...
are of a staging type as well as in the monocrystals of FCC pure metals [8]. However as it has been established in the present work in the alloy the concrete type of staging depends significantly on the monocrystal orientation.

\[ \frac{d\tau}{d\varepsilon} \times 10^{-1}, \text{MPa} \]

![Figure 2](image)

**Figure 2.** Behavior hardening coefficient with deformation for different orientations of the deformation axis alloy single crystals Ni₃Fe.

### 3.2. Dislocation substructure diagrams

The dislocation substructure diagrams represent the dependencies of the volume fraction (Pᵥ) of every observed substructure on the deformation degree. Figure 3 shows the corresponding diagrams for the monocrystals with the orientations [1.8.12] and [011]. On the figures one sees that as the deformation develops at each its stage in the crystal volume one substructure type is actively formed and its volume fraction increases while the fraction of the other decreases. Formation of every new substructure type is connected with the appearance of new stage of hardening on the yield curve.

![Figure 3](image)

**Figure 3.** Depending on the volume fraction of the substructures (Pᵥ) on the degree of deformation for [1.8.12] - (a) and [011] - (b) single crystals studied alloy. Legend substructures: curve 1 - initial chaos; 2 - pile-ups and multipoles; 3 - flat and quasiplanar grid; 4 - three-dimensional network; 5 - three-dimensional grid with misorientation; 6 - net - cellular substructure pa. Dashed lines are deformation stage, \( \varepsilon \) - the degree of deformation.

So in [1.8.12] monocrystals the following transformation chain is implemented: initial chaos → pile-ups and multipoles → plane and quasi plane net → three-dimensional net without disorientations →three-dimensional net with misorientations corresponding to the succession of the deformation stage change: \( \Pi_1 \rightarrow \pi \rightarrow \Pi_2 \rightarrow \Pi_3 \rightarrow \Pi_4 \). Every part in the substructure transformation chain, i.e. every following substructure needs for its formation new acting slipping system which had not taken part in the formation of the previous substructure. Inclusion into deformation of a new slipping system and the appearance of new dislocation interactions connected therewith changes the behaviour of the deformation hardening coefficient: a new stage of work hardening originates. Succession of inclusion into deformation of the slipping systems: primary → conjugated → critical → cross corresponds to the...
above said sequence of deformation stage changes in the monocrystals [1.8.12]. New substructure generation occurs when the developing substructure volume part reaches its maximum and the substructure being prior to it disappears (Figure 3a).

It should be pointed out that the substructure diagram for the monocrystals with orientation [011] is more complex (Figure 3b) than that for the orientation [1.8.12]. This complexity lies in the fact that the three-dimension dislocation net (curve 3) develops at all stages of work hardening.

This depends on the formation of two systems layers with higher dislocation density at the beginning of deformation. Presence of the volume net at the stage II₁ corresponds to the cross sections of the dislocation layers. Aside from that the laws of substructure volume parts changes determined for the orientation [1.8.12] are valid in this case. Correlation of the substructure change succession with the deformation stage change succession also follows from the diagrams of the Ni₃Fe monocrystal substructure oriented for multiple slipping (Figure 4). Such correlation was also observed in Ni₃Fe and Cu-Al polycrystals [7]. It was established that the completion of every deformation stage is connected with occupation of the most part of the material by the same substructure type.

The results obtained in the given work confirm the established law and also let us to conclude that the completion of every stage may be connected not only with filling the most part of material by the same substructure type but also with escape either of the prior or appearance of a new substructure, or with all three events together.

3.3. Distribution of dislocations

Figure 5 shows the histograms of the distances between the nearest dislocations (ℓ) in the slipping planes for all investigated monocrystals. The histograms were plotted for different monocrystal deformation degrees. One sees that at all monocrystal orientations the distributions ℓ being single-modal from the beginning of the plastic deformation remain the same approximately up to 20% of deformation. With the increase of the deformation degree the distributions ℓ become more narrow that in general testifies to the increase of the net substructure homogeneity during the plastic deformation of the alloy Ni₃Fe with short-range atomic order since more and more dislocations lie at the distances close to the average along the crystal. Meanwhile from the beginning of the plastic deformation the net structure in the crystal-edge distance is inhomogeneous at all investigated axis compression orientations. It can be described as ”composite” consisting from the dense plane dislocation layers with rectangular net built in the three-dimension net substructure.
In this connection it should be interesting to investigate the \( \ell \) value behavior separately in the dense and loose layers. Such investigation was done on monocrystals. The results are given in Figure 6. One sees that during the deformation the form of dislocation distribution in the plane net layers – dense layers – is not changed, the average net section size is only changed (Figure 6a). Consequently, for the net structure with “rectangular” net section form in the deformation degree interval where it is formed has the principle of similarity. In the three-dimension dislocation net at small deformation degrees the form of the distribution \( \ell \) (Figure 6b) differs from that in the layers with the plane net. If in the plane net layers it is exponential within the whole investigated deformation degree interval, at the stage II in the volume net the distribution \( \ell \) is close to the logarithmically normal and with the deformation evolves to the exponential one. By the beginning of the stage III the distribution \( \ell \) became practically similar for both net substructure types (Figure 6).

3.4. Scalar dislocation density
The average scalar dislocation density \( <\rho> \) is the most common parameter characterizing the dislocation structure. Figure 7 shows the \( <\rho> \) dependencies on the deformation degree for four investigated Ni\(_3\)Fe monocrystal orientations. It is seen that in all cases the \( <\rho> \) value is monotonically increased with the deformation according to the same law. The differences have qualitative character. As it follows from the comparison of the corresponding curves \( <\rho> - \varepsilon \) (Figure 7) and \( \tau - \varepsilon \) (Figure 1), in a number of monocrystal orientations [1.8.12], [011], and [001] the following correlation is revealed: the higher monocrystal orientation symmetry the larger the dislocation accumulation rate and the value of the given shear stress. This is evidence of an important role played by the dislocation accumulation process in the formation of the flow stress.

4. Conclusion
1. The change in Ni\(_3\)Fe monocrystal orientation from [1.8.12] → [011] → [111] → [001] in the main does not influence on the types of the structures forming in the local volumes but results in displacement of their formation start sideward smaller deformation degrees. This correlates with displacement in the crystals with the orientations [011], [111] and [001] in the same direction of the start of corresponding deformation stages. Identical nature of the deformation curve stages in the
crystals with the orientations [1.8.12] and [011] is explained by the fact that in [1.8.12] the second slip plane enters the deformation early (at the stage $I_1$).

![Figure 7](image_url)

**Figure 7.** Dependence of the mean dislocation density $<\rho>$ the degree of deformation ($\varepsilon$) for single crystals of the alloy Ni$_3$Fe.

2. Influence of the monocrystal deformation axis orientation on the rate of dislocation accumulation was established. The monocrystal orientation change in the direction of the increase of the number of equally loaded octahedron slipping systems (1→ 4 → 8) leads to the increase of scalar dislocation density accumulation rate. This dependence correlates with the $\tau$ – $\varepsilon$ curve behaviour in the orientation series [1.8.12], [011] and [001].

3. In the Ni$_3$Fe monocrystals oriented for single slip one sees the limiting value of the scalar dislocation density in the inhomogeneous parts of the net structure which remains practically invariable within the whole investigated deformation interval. Reaching equality of the average scalar dislocation density means the transition to the stage III.

**References**

[1] Sastry S M L and Ramaswami 1980 *J. Mater. Sci. Eng.* **43** 2 231-234
[2] Karnthaler H P and Schugert B 1980 *Proc. 5th Int.Conf. Strength Met. And Alloys (Aachen)* **1** 205-210
[3] Starenchenko V A, Kozlov E V, Solov'eva Yu.V, Abzaev Yu. A and Koneva N A 2008 *J. Mater. Sci. and Eng.* **483** 179-183
[4] Teplyakova L A, Kunitsyna T S and Koneva N A 2014 *Adv. Mater. Res.* **1013** 54-61
[5] Teplyakova L A, Kunitsyna T S., Koneva N A and Kozlov E V 2004 *J. Bulletin of the Russian Academy of Sciences: Physics* **68** 10 1629-1634
[6] Teplyakova L A and Kozlov E V 2005 *J. Phys. Mesomech* **8** 57-66
[7] Koneva N A and Kozlov E V 1991 *J.Proc. of Higher Education. Phys.* **34** 56-70
[8] Honeycombe R W K 1972 *The Plastic Deformation of Metals* (Moscow: World) p 408