LOOK ACADEMIC PUBLISHERS
OPEN ACCESS

IEJME — MATHEMATICS EDUCATION
2016, VOL. 11, NO. 6, 1563-1576

Dislocation Structure Evolution during Plastic Deformation of Low-Carbon Steel

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ABSTRACT

In this paper, the regularities of structure formation in low-alloyed carbon steels are analyzed. They coincide to a large extent with the general views on the effect of strain degree on the evolution of deformation structure. In ferrite grains, not only the qualitative picture of changes, well known for Armco iron, is repeated, but also the quantitative values of strain corresponding to a change in the structural state are repeated as well. When investigating samples of a ferritic-pearlitic steel, it is found that structure formation in pearlite essentially lags behind structural changes in ferrite grains, and this delay is observed at all stages of deformation. An important feature of structure formation in pearlite is crack nucleation in cementite, accompanied by dislocation pile-up in the ferrite interlayers of pearlite. Using the method of dislocation dynamics, the relationship between structural transformations and the parameters of strain hardening is analyzed. It is demonstrated that the proposed method of computer analysis reflects well the processes taking place in a material during plastic deformation. The character of the theoretical curve of strain hardening is determined by the dislocation structure that forms in a material at various stages of deformation.

KEYWORDS
Low-alloyed carbon steels; strain degree; evolution of dislocation structure; strain hardening; method of dislocation dynamics

ARTICLE HISTORY
Received 21 August 2015
Revised 5 February 2016
Accepted 9 May 2016

Introduction

The deformation technology is one of the most promising ones from the point of view of producing three-dimensional nanostructured articles of commercial dimensions with a high level of strength (Firstov & Rogul, Shut, 2009; Valiev & Zhilyaev, Langdon, 2014; Sahin & Deniz, 2016). The structural studies performed on pure metals (Trefilov et al., 1987) have made it possible to

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obtain a generalized picture of structural transformations taking place during plastic deformation. The established relationship between the structural changes and mechanical properties of materials subjected to deformation enables revealing the physical nature of strain hardening and identify the ways to create materials with superior strength by means of deformation (Valiev et al., 1988; Utyashev & Raab, 2013).

Such ways are connected, on the one hand, with the optimization of the available deformation processes and development of new ones, and, on the other hand, with the deformation of structural alloys with an enhanced strength, which will allow for combining structural strengthening of a chemical nature with dislocation mechanisms of strengthening.

Rolling refers to monotonic deformation actions in the process of plastic treatment (Beigelzimer et al., 2003). For instance, during the fractional (about 5% per pass) rolling of Armco iron, the formation of three main types of dislocation structure was revealed (Trefilov et al., 1987; Firstov et al., 2004). At small strains (~0-15%, monotonic deformation), chaotically distributed dislocations are observed (Figure 1a); at medium strains (~15-60%, «quasi-monotone» deformation), a weakly misoriented cellular substructure is observed (Figure 1b); and at large strains (>60%, «non-monotonic» deformation), a misoriented cellular structure is observed (Figure 1c).

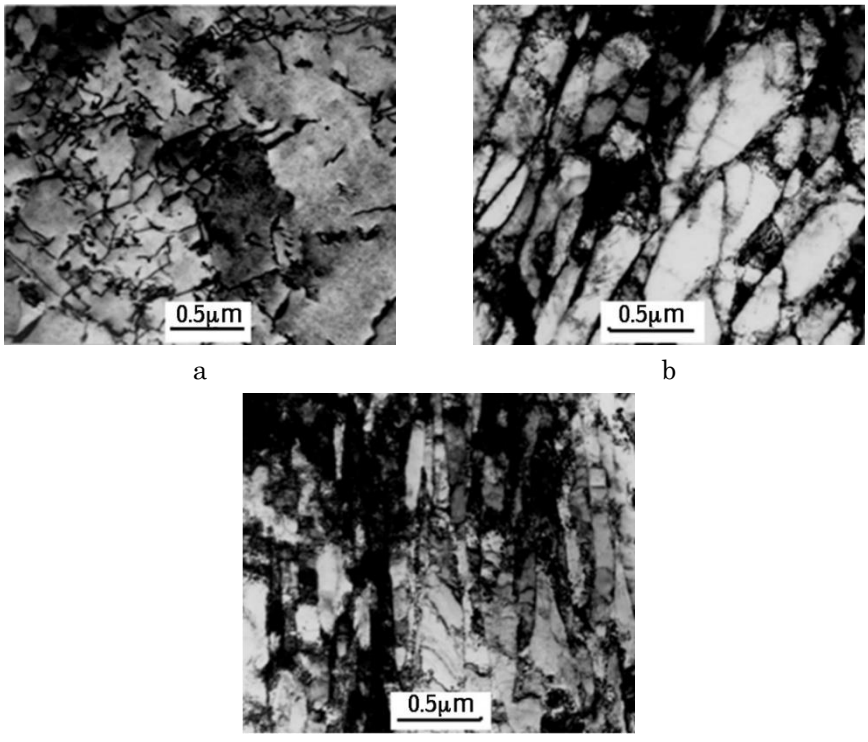


Figure 1. Evolution of the dislocation structure in Armco-iron under deformation: a) dislocation forest, b) weakly misoriented cellular substructure, c) misoriented cellular substructure (Goryachev, 1984).

The boundaries of structural states depend on the deformation conditions (temperature, strain degree) and a material's structure (crystallographic structure, stacking fault energy, grain size, etc.).

The dislocation theories of strengthening are underlined by models establishing a relationship between dislocation density and stress (Goryachev, 1984). In Taylor's duplication theory of strengthening, one proceeds from the assumption that long-range stress fields are the sole source of strain hardening. Since the periodicity in the variation of internal stress in a material is $L=1/\rho^{1/2}$, where L is the average distance between dislocations, the dependence of additional flow stress on dislocation density takes the following form, in accordance with Taylor's theory:

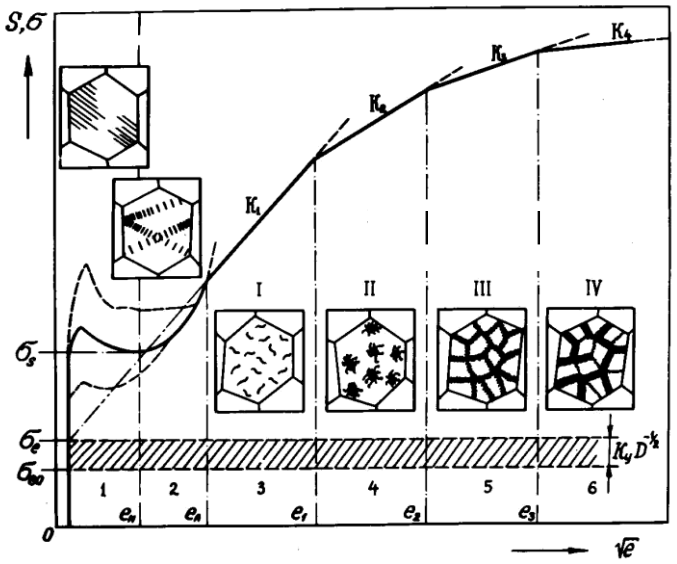
$$\tau = \tau_0 + \frac{Gb}{2\pi K_T}\sqrt{\rho}\,, \qquad (1),$$

where ρ is the density of dislocations lying in the slip plane; K_T is a constant; τ_0 is flow stress. Taking into account the linear relationship between strain and dislocation density, a typical curve of strain hardening of a polycrystalline material is described by a parabola and is given by:

$$\sigma = \sigma_0 + Ke^{1/2}, \qquad (2),$$

where K is the strain hardening coefficient. Variation in the character of deformation structure (from forest dislocations to weakly-misoriented and misoriented cells) influences the strain hardening coefficient at different stages, but leaves the general form of equation (1) unaltered.

The works (Trefilov et al., 1987; Podrezov & Firstov, 2006) have revealed that analysis of strain hardening curves in the coordinates σ–$e^{1/2}$ demonstrates a stage character of the hardening curves, since the curves have inflections to which, according to structural studies, correspond changes in the dislocation structure type.



Fifure 2. Diagram demonstrating the structural sensitivity of the strain hardening curve for bcc metals (Trefilov et al., 1987).

According to the model of strain hardening, the stress-strain curve in bcc metals is described by a parabolic relation (Trefilov et al., 1987; Goryachev, 1984; Podrezov & Firstov, 2006). Such a model enables making a physical interpretation of the curve σ-e, understanding the physical meaning of hardening coefficients and analyzing the effect of external and structural factors on the regularities of strain hardening.

Due to the fact that the most commonly used structural alloys are carbon steels, the aim of the present work is to study the mechanisms of creating deformation structures in the process of monotonic and non-monotonic deformation, with a view to optimize the technology of producing nanostructured states in steels.

Methods

In this work, the evolution of deformation structure in the ferritic-pearlitic steel 20Cr was investigated depending on the degree of preliminary monotonic strain. The initial samples were subjected to deformation by rolling (Rosenberg et al., 1971), at room temperature from different initial thicknesses to the same final size of the rolled sheets – 4.5 mm. The logarithmic strain of the rolled samples was found using the formula e = ln (hi/hf), where hi and hf are, respectively, the initial and final heights of a sample, which reached the following values for the studied structural states: 1 – 0.1; 2 – 0.20; 3 – 0.28; 4 – 0.43; 5 – 0.82; 6 – 1.21; 7 – 1.51. The deformation substructure was studied by transmission electron microscopy on a JEM-100 CX device. The results of study of the deformation substructure by transmission electron microscopy are given in figs. 3 – 7.

In addition to the studies of the dislocation structure of the deformed low-carbon steel, the material's mechanical behavior under a load was modeled, taking into account the collective interaction between dislocations. Also, the issues related to the annihilation of dislocations in the case of their chaotic disposition were considered, and the interaction of the walls with individual dislocations under the conditions of interaction and annihilation of dislocation pile-ups was analyzed.

When modeling by the DD methods, the structure elements are randomly located dislocations whose movement occurs under stress acting from other dislocations of the ensemble. The interaction forces are determined taking into account the distance, angle and sign of a dislocation. It is assumed in the model that a dislocation can glide on the slip plane under the action of the stress σ12 or climb under the action of the stress σ11. The process of slip or climb depends on the ratio between the stresses σ12 and σ11. It is assumed that the rates of slip and climb are equal, and there is a linear dependence of the rate on stress. Dislocation annihilation occurs on the condition that the distance between the dislocations is smaller than 2b, b being the Burgers vector. The rate of annihilation is determined as the change in the number of dislocations of the same sign N depending on time: $\dot{N} = dN/2dt$.

Using computer simulation, the law of dislocation annihilation in the absence of friction force was studied, the effect of friction force on the annihilation law, as well as the relation between the total number of dislocations and the number of non-annihilated dislocations under different friction forces, were determined.

Data, Analysis, and Results

Structural Studies During the Deformation of Low-Carbon Steel

The electron microscopy studies have demonstrated that in the structure of the alloy in the initial state (Figure 3), there are present ferrite and pearlite grains with sizes of ≈ 10 μm and ≈ 7 μm, respectively. Pearlite grains (about 30%) consist of cementite and ferrite interlayers. Cementite plates have a thickness of ~ 250 nm, and ferrite layers – ~ 300÷500 nm (Figure 3 b). Cementite is present predominantly in the form of plates, although somewhere there are spheroidal precipitates.

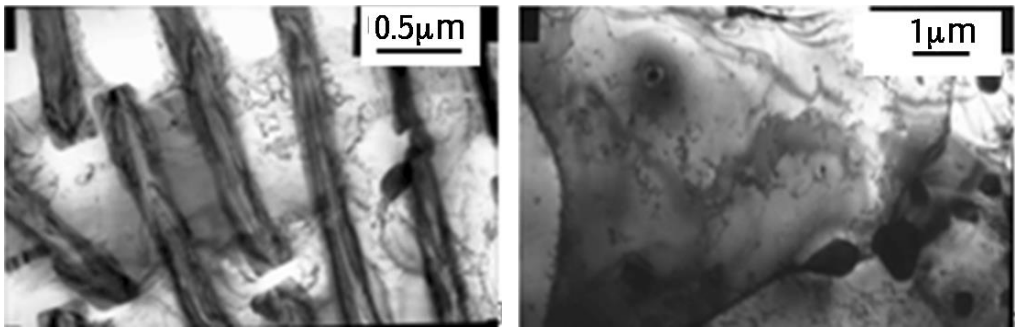


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Figure 3. Transmission electron microscopy (TEM) images showing the structure of the initial material.

Sample straining to e = 0.1 leads to a considerable increase of the dislocation density in ferrite grains, where dislocation pile-ups are formed (Fig. 4 a, b), and practically does not alter pearlite's deformation structure. The results of structural analysis indicate that at the initial stages of rolling, ferrite grains are formed. This is in agreement with the form of the strain hardening curve.

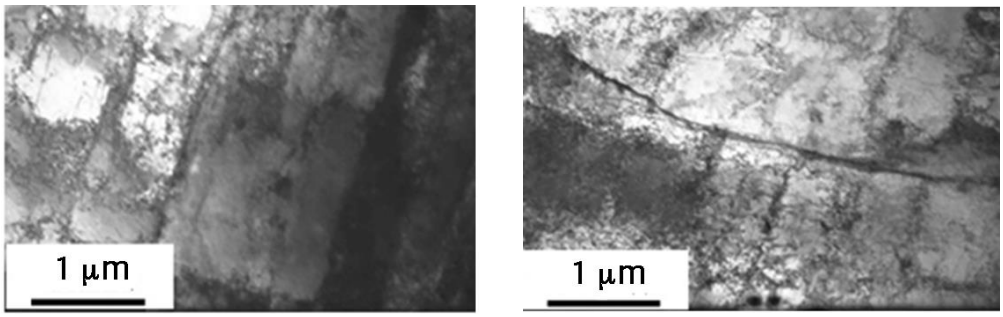

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Figure 4. Transmission electron microscopy (TEM) images showing the structure of the material deformed to e = 0.1.

As the strain is increased to e = 0.2, structural changes are observed in both ferrite and cementite. Here, the structural transformations in cementite essentially lag behind the structural changes taking place in ferrite. In pearlite grains in ferrite interlayers between cementite plates, there are observed dislocation pile-ups. In ferrite grains, dislocation pile-ups transform into a cellular structure. A typical dislocation structure of cell boundaries and the reflections with signs of strands in the microdiffraction patterns indicate that the cells have a predominantly low-angle misorientation. The cell size is 0.4 – 0.6 μm.

In the samples deformed to e=0.28, the deformation interfaces characteristic for a cellular structure appear in the ferrite interlayers of pearlite. The stress concentration during the interaction of these newly-formed interfaces with cementite leads to its cracking and subsequent fracture. In ferrite grains there forms a cellular structure, and the presence of misorientation between the cells is revealed by an analysis of the dark-field images of the structure (Figure 5 a).

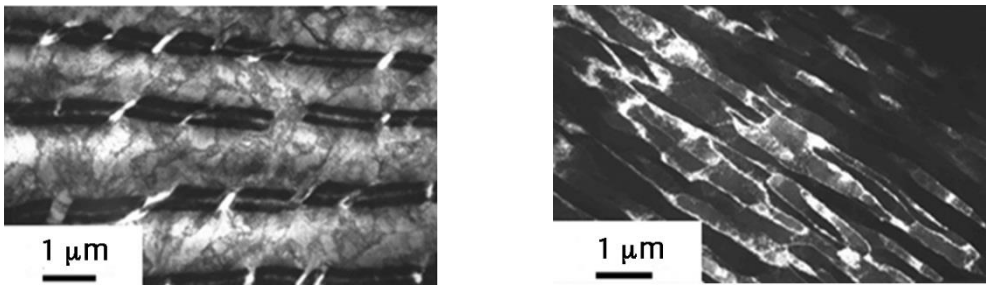

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Figure 5. Transmission electron microscopy (TEM) images showing the structure of the material deformed to e = 0.28, for weakly misoriented cells.

As the strain is increased to e = 0.43, in ferrite grains there starts to form a developed cellular structure, where the cell sizes decrease to a critical size of 0.25 μm. However, the interfaces between the cells remain weakly misoriented, as evidenced by strands in the electron diffraction patterns. In pearlite grains there also form cells, the presence of which provokes cementite fracture due to stress concentration at interphase boundaries.

When the samples are deformed to a strain of e = 0.82, the misoriented cellular structure in ferrite grains becomes more developed, which is assisted by the rotational mechanism of deformation. The activation of this mechanism is evidenced by shearing band-like areas (Figure 6 a) that may be interpreted as a consequence of disclination movement. Note should be made here that in the electron diffraction patterns, reflections with strands, which are characteristic for low-angle structures, prevail. The length of the strands increases as compared with the less deformed states of the alloy, which testifies to an increase of the average misorientation angle (Figure 6 a). A change in the deformation mechanism in ferrite reduces the stress concentration in pearlite grains where, in spite of the presence of predominantly weakly misoriented cells, cracks in cementite disappear (heal) and a partial coagulation of cementite plates occurs (Figure 6 b).

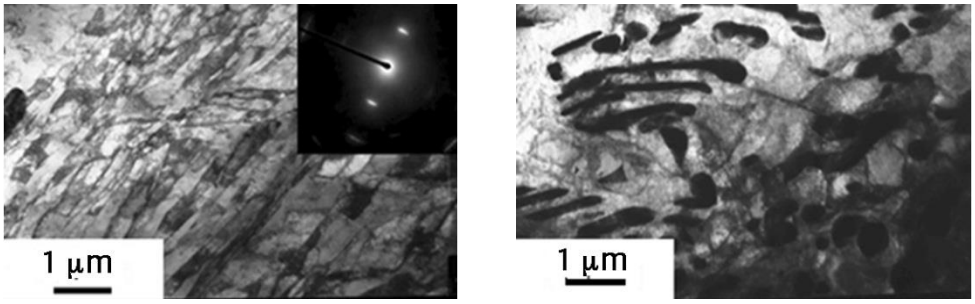

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Figure 6. Transmission electron microscopy (TEM) images showing the structure of the material strained to e = 0.82, for misoriented cells.

The strain e = 1.21, according to the common classification (Rybin, 1986), can be referred to large or developed (non-monotonic (Beigelzimer et al., 2003)) ones. For this strain, the formation of misoriented cellular structures is typical. Structural studies confirm that in ferrite, there form predominantly misoriented cells with an average size of 0.25 μm, reflections with strands in the electron diffraction pattern become mainly point-type, which is characteristic of nano-grained structures. In pearlite the cellular structure evolves slower, and its evolution essentially lags behind the structure evolution in ferrite grains.

In the state deformed most severely, to a strain of e = 1.51, in ferrite grains there forms a deformation-induced nanostructure with a high-angle misorientation, as evidenced by the results of dark-field studies (Figure 7 a) and point reflections in the electron diffraction patterns (Figure 7 a). Under super-high strains, in pearlite grains the first signs of rotational processes are observed: the formation of structures in the form of shear bands (Figure 7 b), where strain concentration promotes cementite cracking.

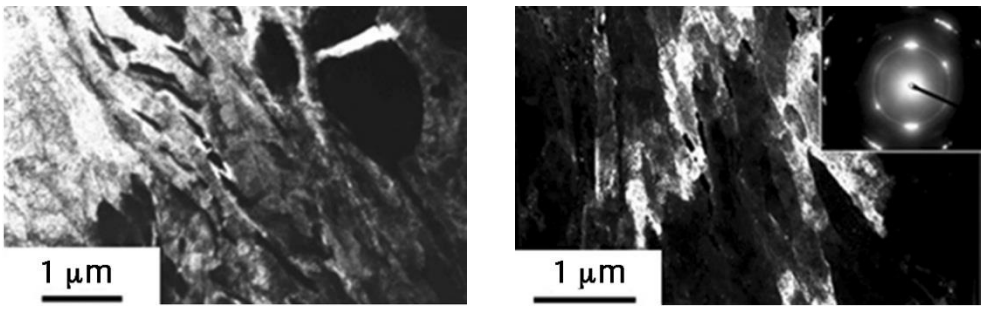

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Figure 7. Transmission electron microscopy (TEM) images showing the structure of the material strained to e = 1.51, with misoriented cells.

Modeling of the Mechanical Behavior of the Deformed Material Using the Dislocation Dynamics (DD) Method

It has been shown that if friction force is absent, the dislocation density ρ has a linear dependence on time: $\rho=(1/\rho_0+\alpha t)^{-1}+\rho_l$, and if this is not the case, then:

$$\rho=(1/(\rho_0-\rho_l)+\alpha t)^{-1}+\rho_l, \quad (3)$$

where ρ_l is the density of non-annihilated dislocations. Calculation of the parameter α has shown that if friction force is absent, this parameter does not

depend on the number of dislocations and equals $\alpha=2\nu_c Gb/L^2$, where ν_c is a coefficient, G is the shear modulus. If friction force is present, this parameter remains invariable only under a small friction force. As the friction force is increased, the value of α independently calculated from equation (3) differs from the results of the computer experiment, which is connected with the small number of non-annihilated dislocations.

The stresses of the interaction between one dislocation and a dislocation wall were calculated. The calculation has shown that in case a dislocation and a wall have the same sign, at the upper and lower edges of the wall there are regions of attraction of the dislocation to the wall. The obtained results are in agreement with the data by V.N. Perevezentsev and co-authors (Sarafanov & Perevezentsev, 2005; Perevezentsev, Sarafanov & Svirina, 2014), according to which, the presence of such regions may promote the concentration of dislocation pile-ups at the edge of disclinations. In case a wall and a dislocation have different signs, at a certain distance from the wall there is a region of unstable equilibrium, which may lead, in the absence of friction force, to the nucleation of a wall with a different sign.

Also, the interaction of two walls consisting of dislocations having the same sign was considered. It has been established that the parameter that determines the minimum equilibrium distance L_0 between the walls is the friction force σ_{fr}. This distance can be derived from the following equation: $L_0=Gb/2\pi\ (1-\nu)\sigma_{fr}$. If dislocations in the walls are contained not only due to the Peierls force, but also due to the additional forces of interaction between a dislocation and impurities, the equilibrium state between the walls can sharply decrease.

This conclusion is confirmed by the results of the work (Danylenko et al., 2009) which has demonstrated, using transmission electron microscopy studies, that when a dislocation nanostructure is formed in the presence of a large amount of impurities interacting with dislocations, the size of cellular structure decreases practically by an order of magnitude. The results of the investigation on the processes of dislocation relaxation and annihilation by DD methods can be used to analyze the phenomena of recovery (static and dynamic). When modeling the structural transformations taking place under an active load, one should add to the considered processes of interaction between dislocations the stage of dislocation nucleation. Therefore, further we shall consider a case when a dislocation structure is formed in the presence of dislocation nucleation sources.

When modeling the evolution dynamics of the dislocation structure in the presence of dislocation sources, at each moment of time we calculated:

1) Stress at the source, as a sum of external stress and the stress from the dislocation ensemble.

2) The current stress components at each dislocation of the ensemble.

3) The dislocation velocity, assuming its linear dependence on stress.

4) New positions of a dislocation, found from the information about the deformation velocity $x_i(t+dt)=x_i(t)+v_i dt$ and taking into account the condition that under $\sigma_{12}>\sigma_{11}$slip takes place, and under $\sigma_{11}\geq\sigma_{12}$ climb takes place.

5) The total strain $\varepsilon=b\Sigma\ v_i dt\ /L$.

6) The movement energy $J=\Sigma\ \sigma_i v_i dt$.

In case forest dislocations are absent, only tangential stresses exert action on the source, and it operates in the mode of generating dislocation pile-ups.

Using software we designed, we calculated the dependencies of the number of dislocations and accumulated strain on time, under different external stresses. It has been established that the number of dislocations in a pile-up increases in a linear fashion as external stress grows, which is in good agreement with Leibfried's theoretical dependence (Ekobori, 1971), calculated for a limiting equilibrium case. It has been demonstrated that the dependence of the number of dislocations in a pile-up on time is sensitive to the boundary conditions (model crystal size).

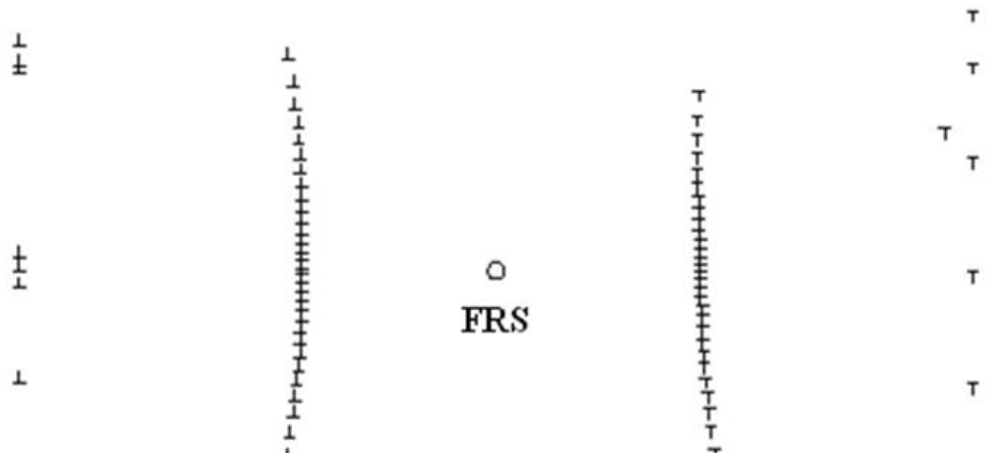
Using a model crystal with a size of 1000 b, the dependencies in the variation of the number of dislocations and strain in a pile-up on time were analyzed. It has been shown that strain depends on the load in accordance with a law close to $\sigma \sim e^{1/2}$, which, in its turn, is in agreement with V.I. Trefilov's (1987) theory of strain hardening.

When constructing DD models, in accordance with (Segurado, Lorca & Romero, 2007; Borysovska & Podrezov, 2006; Borysovska, Podrezov & Firstov, 2007), long-range fields of elastic stresses between individual dislocations were considered and the collective processes of their interaction were analyzed.

Where forest dislocations are present, both tangential and normal stresses exert action on a dislocation source. In accordance with (Borysovska & Podrezov, 2006; Borysovska, Podrezov & Firstov, 2007), in the framework of the dislocation dynamics of a two-dimensional model of infinite edge dislocations, several operation modes of the Frank-Read source (FRS) in the presence of forest dislocations were studied. It has been shown that there are three operation modes of the source (Figs. 8–10):

- when the influence of forest dislocations is not decisive, the source operates in a classical mode of generating dislocation pile-ups, Figure 8;
- generation of dislocation walls, when forest dislocations cause the climb of dislocations emitted by the source, there occurs an avalanche-liken nucleation of dislocations that build walls in the vicinity of the FRS (Figure 9);
- «intermediate mode», when the source operates alternately in the mode of wall generation and in the pile-up mode (Figure 10).

Figure 8. Operation of the Frank-Read source (FRS) in the pile-up mode.



Fifure 9. Operation of the Frank-Read source in the mode of generation of dislocation walls.

Fifure 10. Operation of the Frank-Read source in the alternating mode.

Among the considered modes, of most interest is the mode of generation of dislocation walls, since the formed dislocation configurations can be viewed as a prototype of the dislocations which were theoretically predicted and experimentally observed many times by V.V. Rybin and his co-workers (Rybin, 2002; Orlov, Perevezentsev & Rybin, 1980).

Using a computer experiment, the dependence was calculated between the wall parameters (the number of dislocations in a wall and the wall's length) on the applied stress at various distances of a trial dislocation from the source. It has been demonstrated that under the optimum loading conditions a wall is formed by over 100 dislocations. Since the software enables measuring at the same time the wall's misorientation angle α according to the formula: $\sin(\alpha/2)=b/2D$, where D is the distance between dislocations, we calculated the crystal's misorientation provided by such a wall. The calculation has shown that the crystal's misorientation at different sides of the wall may reach 40-50 degrees, i.e. such a wall has all the signs of a disclination defect.

The dynamics of structural transformations in the crystal was considered for the condition of a simultaneous action of several sources under a constant external stress. In this case, the sources operate periodically either in the mode of wall generation, or in the pile-up mode. Calculations of the dependence of the number of dislocations and strain on time have shown that after a certain period of time, the number of dislocations in the crystal stabilizes at a constant level. At that stage, strain increases in a linear fashion with time, while strain rate settles at a constant level, thus the formal signs inherent in the deformation of a material in the creep mode are realized.

The dislocation dynamics method was used to build a stress-strain curve under an active load. In the model material, where three sources operated simultaneously, stress increased during the model experiment in accordance with the linear law. The studies have shown that under this variant of load, the

dislocation structure transforms successively: under small stresses the dislocation sources do not operate and the material experiences deformation in an elastic manner; as the stress somewhat increases, the sources operate in the mode of pile-up generation in different planes, and there is no dislocation annihilation.

As the stress grows further, there start to form dislocation walls where the number of dislocations gradually increases, and the process of dislocation annihilation takes place simultaneously. As the stress grows even further, the number of dislocations practically stabilizes at a constant level. The estimated dependence of the number of dislocations on stress under a continuous loading and the stress-strain curve are shown in Figures 11 and 12, respectively.

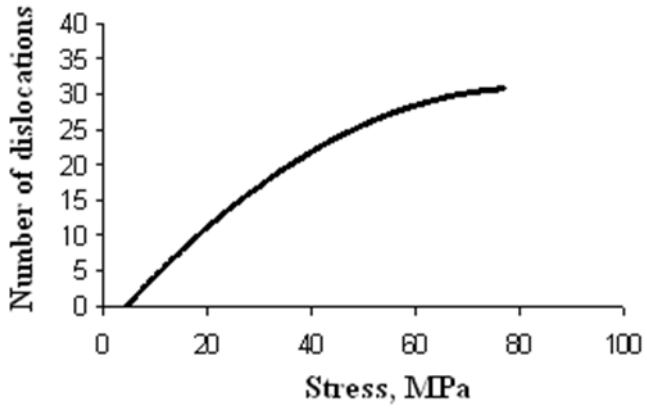


Figure 11. Dependence of the number of dislocations on stress under a continuous loading.

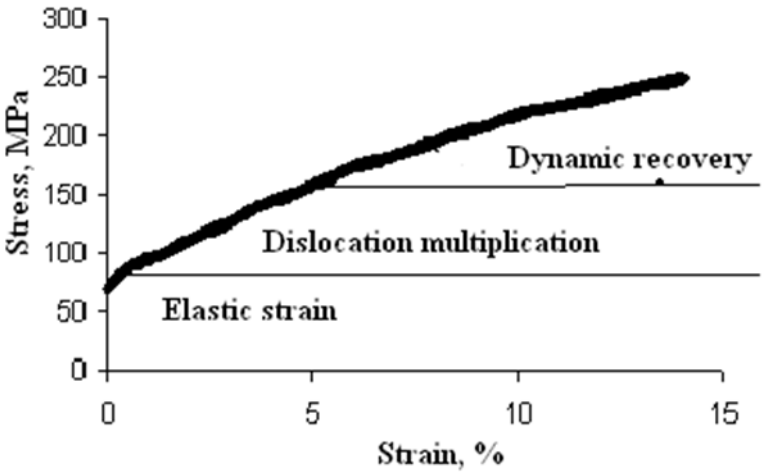


Figure 12. Stress-strain curve.

Note should be made that the character of the strain hardening curve depends on the dislocation structure which forms in the material at different stages of deformation, since the hardening rate is determined by the number of mobile dislocations during each period of time.

The character of the loading curve is in good agreement with the current notions about the sensitivity of hardening rate to the character of the interaction

between dislocations at different states of strain hardening (Goryachev, ,1984). There appear the stage of dislocation multiplication and the stage of dynamic recovery (Figure 12).

Discussions

Thus, the regularities of structure formation in low-alloyed carbon steels coincide to a great extent with the general views on the effect of strain degree on the evolution of deformation structure. In the first place, this concerns a change of structural states in ferrite grains. Here, not only the qualitative picture of the changes, well known for Armco iron (Firstov et al., 2004), is repeated, but also the quantitative values of strain corresponding to a change of the structural states are repeated as well. The microstructure of the samples strained to e=0.1 and 0.2 should be referred to chaotic dislocation structures; and the microstructure of the samples strained to e=0.28 and 0.43 should be referred to weakly misoriented cells. The samples strained to e=0.82; 1.21 and 1.51 have misoriented nanograins in ferrite.

At the same time, note should be made about some features of structure formation in deformed ferritic-pearlitic steels. First, structure formation in pearlite essentially lags behind the structural changes in ferrite grains. This can be explained, taking into account that the microhardness of pearlite grains is about a third higher than that of ferrite grains. Proceeding from the hardening curve of ferritic steel, when the same stress is applied to a sample, pearlite grains will start to deform under the stress that corresponds to a 10-20% plastic deformation of ferrite. This delay remains at all stages of deformation, as demonstrated by electron microscopy studies of the microstructure of the samples after deformation. Second, an important feature of structure formation in pearlite is crack nucleation in cementite in structural states where dislocation pile-up in ferrite interlayers of pearlite leads to an increase in stress concentration in the vicinity of cementite plates.

The stage character of the structural changes and the mentioned features of structure formation in ferritic-pearlitic steels were taken into account when we analyzed the effect of strain degree on the mechanical properties of the material, measured using different testing methods: uniaxial tension, uniaxial compression, hardness testing and crack resistance testing (Danylenko, Podrezov & Firstov, 2015).

Conclusion

1. The regularities of structure formation in low-alloyed carbon steels coincide to a great extent with the general views on the effect of strain degree on the evolution of deformation structure. In ferrite grains not only the qualitative picture of the changes, well known for Armco iron, is repeated, but also the quantitative values of strain corresponding to a change in the structural states are repeated as well. In the samples strained to e=0.1 and 0.2, there forms a chaotic dislocation structure; in the samples strained to e=0.28 and 0.43, there form weakly misoriented cells; and in the samples strained to e=0.82, 1.21 and 1.51, there forms a structure with misoriented nanograins in ferrite.

2. Structure formation in pearlite essentially lags behind the structural changes in ferrite grains – pearlite grains start to deform under a stress

corresponding to 10-20% plastic deformation of ferrite – and this delay remains at all stages of deformation. An important feature of structure formation in pearlite is crack nucleation in cementite accompanied by dislocation pile-up in the ferrite interlayers of pearlite.

3. The microstructure of the samples strained to e = 0.1 and 0.2 should be referred to chaotic dislocation structures; and the microstructure of the samples strained to e = 0.28 and 0.43 should be referred to weakly misoriented cells. The samples strained to e = 0.82, 1.21 and 1.51 have misoriented nanograins in ferrite.

4. An increase in the stress of lattice friction with decreasing temperature, or caused by the interaction of impurities with dislocations in the 20Kh steel, leads to a significant reduction in the size of nanograins of deformation origin.

5. Using the method of dislocation dynamics, the relationship between structural transformations and the parameters of strain hardening has been analyzed. It has been demonstrated that the proposed method of computer analysis reflects well a stage character of the processes taking place in the material during plastic deformation. The character of the theoretical curve of strain hardening is determined by the dislocation structure that forms in the material at various stages of deformation.

Acknowledgments

G.I. Raab and L. N. Shafigullin acknowledge gratefully the funding through the Russian Government Program of Competitive Growth of Kazan Federal University.

Computer modeling using the dislocation dynamics (DD) method was carried out due to the support from the Russian Science Foundation grant (project No. 14-19-01062), allocated to Ufa State Aviation Technical University.

Yu. N. Podrezov, M. I. Danylenko and K. M. Borysovska would like to acknowledge the support from the Ukraine-Russian Science Foundation grant (project Ukr_a 0890429).

G.N. Aleshin acknowledges gratefully the financial support from the Ministry of Education and Science of Russia through project No. 11.729.2014K.

Disclosure statement

No potential conflict of interest was reported by the authors.

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