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The influence of the dislocation distribution heterogeneity degree on the formation of a non-misoriented dislocation cell substructures in f.c.c. metals

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Abstract. Dislocation loops emitted by Frank-Reed source during crossing dislocations of the non-coplanar slip systems are accumulates jogs on the own dislocation line, resulting in the deceleration of the segments of dislocation loops with high jog density. As a result, bending around of the slowed segments the formation of dynamic dipoles in the shear zone occurs. In the present paper we consider formation mechanism of non-misoriented dislocation cell substructure during plastic deformation of f.c.c. metals and conclude that the increase in the degree heterogeneity of dislocation distribution leads to an increase in the jog density and reduce the mean value of arm dynamic dipoles.

1. Introduction

Non-misoriented dislocation cell substructure (NMDCS) was the first experimentally observed dislocation structure [1] and attracted the attention of researches due to its contribution to the strengthening of the material [2 – 4]. It is observed as bright spots, surrounded by lots of dark stripes that forms cell boundaries. Cell boundaries may contain areas with misorientations of no more than half a degree [4].

According to the modern concept of cell structures, non-misoriented dislocation cell substructures assumed as heterogeneous substructure, dislocations of which mostly located in the walls of finite thickness, consisting of dipoles and multipoles hindering movement of shear-forming dislocations [4].

It is known that f.c.c. metals with high energy (more than 60 MJ/m^2) stacking fault characterized by cellular substructure with blurred cell walls under moderate or impulse loads. With decreasing of this energy the tendency of cell formation become weaker and dislocation plexus become more observable. Structure is dominated by twins and stacking faults at low energies (less than 25 MJ/m^2) [5, 6].

Study of dislocation structure of f.c.c. single crystal copper oriented for single slip [7] showed that crystals under small deformations have free strongly curved primary dislocations as well as dipole and multipole configurations, consisting mainly of screw dislocations. Screw dislocations and dipoles were observed either rarely or not at all, what allows to conclude that they are quickly annihilating by cross slip [8].

In the beginning of strain, the dislocation reactions resulting to formation of dislocation plexus uniformly over the entire sample from which the walls of cells are formed in single crystals oriented for multiple slip [8– 14].

In the copper even at low stresses and strains $\tau \approx 10\,\mathrm{Pa}$ cellular structures with flat rounded cells, lying in the planes perpendicular to the axis of tension, are formed. Average area of cells that are almost freed of dislocations, decreases with increasing of stress measured in MPa according to the law $25.5\tau^{-2}$. Average cell diameter d_C is always smaller, then the length of the slip traces. Since the length of the slip traces has the same order as the diameter of shear zone D, then for single crystal copper at room temperature $D \approx 4d_C$ [9], i.e. four cells are formed in the shear zone. With increasing stress, the dislocation density in the cell walls increases proportionally $\tau^{2,3}$ with the proportionality coefficient that depends on the orientation of the sample [9].

When using the cyclic strain, the cells with more regular shape are formed and their walls are built of more correct and less intertwined dislocation structures [15]. On the basis of the observation was concluded that the plastic strain is concentrated inside the cells, and the saturation state inside the cells there are groups of free dislocations with generally screw orientation, as well as the vacancy dipoles with arm of $3.5\,\mathrm{nm}$ [15].

In copper polycrystals for an average diameter of dislocation cells were found: $d_C = 16\rho^{-1/2}$ and $\tau = 10.5Gb/d_C \approx 0{,}66Gb\rho^{1/2}$ [16]. Inverse proportionality of the shear stress τ to the average diameter of cells was found in other single and polycrystalline f.c.c. metals. For nickel $d_C = (7\ldots12)\rho^{-1/2}$, moreover proportionality coefficient is little affected by temperature and deformation degree, and close to the values of other pure metals [17].

Thus, in metals and alloys cells are characterized by average diameter $d_C = (2\ldots16)\rho^{-1/2}$ and wall width $h_C = (0{,}3\ldots0{,}5)d_C$ $h_C = (6\ldots80)\cdot10^{-5}$ at $\rho = 10^8\,\mathrm{sm}^{-2}$.

Consequently, the diameter of the cells corresponds to the mean free path of screw segments. Therefore, the formation of the cell structure may be linked with the evolution of the dynamic multipole structure. With increasing strain cells are grinding, and their average size is reduced to value of $0.2\,\mu\mathrm{m}$.

Formation and evolution of NMDCS studied both experimentally, and by mathematical modeling [18 – 21]. The main quantity characterizing the evolution NMDCS with increasing degree of plastic deformation, is a dislocation density of the dynamic dipole configurations ρ_d. In addition, mathematical models of plastic deformation include NMDCS characteristics as an equation parameters, such as the average value of the dipole arm h_d, the mean free path ℓ_d of a screw dislocation with jogs and the average shear zone area S_D, i.e. the average area swept out by shear-forming dislocations emitted by Frank-Read sources.

For convenience, the dipoles are considered to consist of elementary dipoles with length ℓ_d and for the output of dipoles accumulation intensity number of elementary dipoles n_d is used.

To construct a mathematical model firstly we need to answer the following questions. What is the resistance to movement of the screw orientation of the segments have jogs? How many jogs on the segment with screw orientation is necessary for a significant slowdown of the segment? What is the average value ℓ_d of path that run segments of shear-forming dislocations having jogs with screw orientation before bending around adjacent segments with lower jog density? How many elementary dipoles are formed in the area S_D after the passage of a dislocation loop? What is distribution function for arm of dynamic dipoles? What is the intensity of the dynamic dipole generation? What is the annihilation rate of the thermodynamically stable dynamic dipoles under the influence of flow deformational point defects? What is the intensity of point defects generation due to the dissociation of the thermodynamically unstable dipoles with a small dipole arm? What effect does the reduction of the shear zone area S_D with increasing degree of deformation on the formation of NMDCS?

2. Formation of non-misoriented dislocation cell substructure

In the first papers on the modeling of evolution NMDCS assumed that the deceleration and self-locking of screw segments of dislocation loop after the run for a distance ℓ_d because of the increase in the jog concentration it leads to a bending around the adjacent more mobile segments.

In the process of bending around as a result of run edge segments the new segments with a screw orientation are formed, which also bending around after run of about the same distance ℓ_d. As a result, within the shear zone the system of dipole and multipole dislocation configurations occurs. NMDCS formed due to the transformation of the dipole configuration system and disappears due to the dissociation and annihilation of dipoles. The dislocation density in the cell walls is the same as ρ_d, while the dislocation density inside the cells - is part of ρ_d determined by not transformed dipoles remaining at the time of observation.

Equating work of screw segments on the drawing of jogs $\tau_j b\,\mathrm{d}S_D^s$ to the total energy of generated point defects $0.5(U_i^f + U_\upsilon^f)\,c_j\,\mathrm{d}S_D^s/b$, where U_i^f and U_υ^f - formation energy of interstitial atoms and vacancies, respectively, we get strain $\tau_j = 0.5c_j\,(U_i^f + U_\upsilon^f)/b^2 \approx 0.25Gbc_j$ that necessary for nonconservative drawing of jogs [18 – 21].

The value of ℓ_d depends on the jogs concentration c_j, because stopping of the screw segment occurs when strain $\tau_j = 0.25Gbc_j$ that need for drawing of jogs becomes larger than effective strain $\tau_{eff} \approx \alpha_{eff} Gb\rho^{1/2}$ that spreads the loop. Since the concentration of jogs c_j does not exceed the value $\beta_j\xi\rho\ell_d$ obtained by integration of jogs generation rate $c_j \approx \int_b^{\ell_d} \beta_j\,\xi\rho_m\,\mathrm{d}x \approx \beta_j\xi\rho_m\,\ell_d$, then basis on the inequalities $0.4\rho^{1/2} \le 0.25c_j \le 0.25\beta_j\xi\rho\ell_d$ it follows that value ℓ_d is not less than $4\alpha_{eff}\beta_j^{-1}\xi^{-1}\rho^{-1/2} \approx (2\ldots8)\rho^{-1/2}$ on condition of $\alpha_{eff} = 0.1\ldots0.4$.

Due to the movement of a dislocation loop $n_d = 2F_d\ell_d^{-2}S_D^s$ elementary dipoles are formed, all the dipoles consist of them. Next apply $n_d = 42$; $F_d \approx 0.3$; $\ell_d = 8\rho^{-1/2}$. In this case on the segment with length ℓ_d there is on average $c_j\,\ell_d \approx 14$ jogs.

If N of dislocation sources per unit of volume emit portion on the average of Δn dislocations loops during time Δt, then shear plastic deformation a will increase by the amount of $\Delta a = S_D b\,n\,N$. Since dipole consists of two dislocation segments, then with increasing shear strain at Δa density of dislocation that form dynamic dipoles during one elementary act of segment-source, increases by the amount of $\Delta\rho_d = \Delta\rho_d^\upsilon + \Delta\rho_d^i = 2n_d\,\ell_d\,\Delta n\,N$.

Consequently, the dislocations in the dynamic dipole configurations of interstitial and vacancy types accumulates with intensity of $G_d = 2n_d\ell_d S_D^{-1}b^{-1}$.

Considering the intensities of dynamic dipole generation with interstitial G_d^i and vacancy G_d^υ types equal between each other we get

$$G_d^i = G_d^\upsilon = 0{,}5G_d = F_d S_D^s S_D^{-1}\ell_d^{-1}b^{-1} \approx 0{,}125F_d b^{-1}\rho^{1/2}. \quad (1)$$

Where ρ_d^i, ρ_d^υ - dislocation density in dynamic dipole configurations of interstitial and vacancy types, respectively.

Dislocations that forms vacancy dipoles, annihilates by the climbing as a result of the interstitial atom deposition, whereas dislocations, that form interstitial dipoles, annihilates by climbing as a result of monovacancies and bivacancies deposition.

Annihilation rate A_{id}, $A_{1\upsilon d}$, $A_{2\upsilon d}$ of point defects during their deposition at the edges of extraplanes of dipoles have form of:

$$A_{id} = \rho_d^{\upsilon} D_{id}\ c_i\ ,\ A_{1\upsilon d} = \rho_d^{i} D_{1\upsilon d}\ c_{1\upsilon}\ ,\ A_{2\upsilon d} = \rho_d^{i} D_{2\upsilon d}\ c_{2\upsilon}\ . \quad (2)$$

Where D_{kd} - diffusion coefficients, c_i, $c_{1\upsilon}$, $c_{2\upsilon}$ - concentrations of point defects (interstitial atoms, mono- and bivacancies respectively).

Annihilation rate of the dipoles under the influence of ping defects have form []:

$$A_{di} = w_d^i A_{id} < h >^{-1} b^{-1}\ ,\ A_{dk} = w_d^k A_{kd} < h >^{-1} b^{-1}\ ,\ k = 1\upsilon,\ 2\upsilon\ . \quad (3)$$

Where w_d^i, $w_d^{1\upsilon}$, $w_d^{2\upsilon}$ - ratio of total surface area of the tubes with radius b around dislocations, that forms dipoles, to total surface area of all sinks for point defects of every type.

3. Influence of the degree of the heterogeneity of the distribution of dislocations on the NMDCS formation

The value ℓ_d depends on the jog concentration c_j, so the accumulation of dislocations in the dynamic dipole configuration depends significantly on the distribution by dislocation sign of non-coplanar slip systems, crossed by the screw segments.

The dislocations intersection of non-coplanar slip systems leads to the fact that the segments, bending around the decelerating segment of screw orientation, turn out to be in planes different from the original slip plane of the shear-forming dislocation. The distance from the original slip plane where the bending around segments are moved away. It depends on its swept out area and distribution of the jogs-forming dislocations in this area.

The minimum distance equal to the distance $\sqrt{6}b/3$ between adjacent planes of octahedral slip, however it is possible that the enveloping segments will meet on one plane, after that the dipole is not formed or the arm dipole can be considered to be equal to zero.

The maximum distance will be reached, if the enveloping segments cross all the noncoplanar shear zone dislocations, and it will be equal to Δnb of the product of the number of emitted loops per module of the Burgers vector. In the random distribution of the "forest" dislocations the appearance of a dipole with a maximum arm is much less likely than the appearance of a dipole with a minimum and even average lever.

The area occupied by one dipole, is deduced from a ratio $\gamma_d \ell_d^2 \approx S_D^s n_d^{-1} = 0{,}5\ell_d^2 F_d^{-1}$ of the area gripping by the screw segments to the number n_d of elementary dipoles.

Average arm dipole is expressed as the product of the area $< h >= \left|\beta_j^+ - \beta_j^-\right| \xi\rho\,\gamma_d \ell_d^2\,\sqrt{6}b/3$ per one dipole, on the difference between the fractions of jog-forming dislocations with a different sign, on the "forest" dislocations density $\xi\rho$ and the distance $\sqrt{6}b/3$ between adjacent slip planes.

In the entire material volume the values β_j^+ and β_j^- are approximately equal, but in the area per one dipole, they may vary. It is clear that $\beta_j^+ + \beta_j^- = \beta_j \approx 0.43$ - the fraction of the "forest" jog-forming dislocations.

If dislocations of only one sign are crossing, the maximum arm dipole of the dipole is: $h_{\max} \approx 0.43\xi\rho\,\gamma_d \ell_d^2\,\sqrt{6}b/3$.

Suppose that the function graph of distribution function for arm of dynamic dipoles is a straight line cutting-off on the x-axis a segment whose length is $h_{\max}$, then the density function is restored as follows:

$$f_h(x) = 2h_{\max}^{-1}(1 - xh_{\max}^{-1}) , \tag{4}$$

and the mathematical expectation is: $< h >= h_{\max}/3$.

Given that, $\gamma_d = 0.5F_d^{-1}$, $F_d \approx 0.3$, $\ell_d \approx 8\rho^{-1/2}$ for the maximum value of the dipole lever from the dislocation in dynamic dipole configurations and dislocation fragments we get $h_{\max} \approx 0.43\xi\rho\,\gamma_d \ell_d^2 \sqrt{6}b/3 \approx 18b$, and for average value - $< h >\approx 6b$.

At the intersection of dislocations with the opposite signs the jogs that can be annihilated, moving along the dislocation line are formed on the screw segments. This reduces the deceleration force of shear-forming dislocation, increases ℓ_d and decreases the number of generated elementary dipoles. If ℓ_d is close to the shear zone diameter, then the dynamic dipoles are not formed.

The jogs fraction w_j that can annihilate is determined by their distribution on screw segments by the sign. The value w_j is being decreased with the increasing of the excessive density of dislocations creating a local disorientation. At the intersection of the area with the excessive density of dislocations on a segment by screw segment, the jogs of the same sign are formed, that lead to a significant inhibition of the segments, reduce ℓ_d and increase the number of the generated elementary dipoles. Furthermore, by virtue of the fact that w_j is evidently proportional to $\left|\beta_j^+ - \beta_j^-\right|$, then with the excessive dislocation density increasing, the maximum value of the dipole arm is reduced.

Dipole with an arm of a few interatomic distances that are thermodynamically unstable, so a dipole arm decrease leads to a rate dissociation of interstitial dipoles and annihilation of vacancy dipoles under the influence of the forming interstitial atoms. This fact seems to be the reason that with increasing of the strain degree and excessive dislocation density the NMDCS is a small factor in the hardening by the time of fragmented substructure formation is not observed.

4. Summary

It is shown that with increasing degree of heterogeneity of distribution of dislocations due to the formation of excess dislocation density, the following occurs: decreasement in the mean free path of screw segments, increasement in number of elementary dipoles and decreasement in the dipole arm. As a result of the dissociation of the interstitial dipoles with a small arm the annihilation of dipoles becomes more intense and rapid disappearance of the non-misoriented dislocation cell substructure occurs.

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