Estimation of the shear zone size in FCC – single crystals based on the model of dislocation interactions

V A Starenchenko¹, R I Kurinnaya¹, D N Cherepanov¹, M V Zgolich¹ and O V Selivanikova²
¹Tomsk State University of Architecture and Building, Department of Higher Mathematics, Tomsk, 634003, Russia
²National Research Tomsk Polytechnic University, Department of Physical and Power Plants, Tomsk, 634050, Russia

E-mail: riklaz@mail.ru

Abstract. The main objective of the mathematical modeling of a shear plastic strain is estimation of the shear zone size. The paper is devoted to refinement of estimations of the shear zone size based on the model of dislocation interactions proposed by the authors. It is assumed that shear-forming dislocation loops, emitted by the dislocation source, are stopped by strong dislocation barriers that arise from the interaction of segments of expanding dislocation loops with reacting dislocations of non-coplanar slip systems. The formed barriers hinder further expansion of dislocation loops and, as a result, form the boundary of the shear zone. A refined estimation of the shear zone size has been obtained.

1. Introduction

Physical understanding of plastic strain of crystalline materials had arisen as a result of overcoming the contradictions between theoretical concepts and experimental results. For example, the crystal strength calculated based on the understanding of simultaneous breaking of atomic bonds in a glide plane was a thousand times greater than the actual strength. This problem was solved by introducing the notions of the dislocation, the displacement of which leads to breaking of atomic bonds along the dislocation line only. However, this case also includes a contradiction connected to the fact that the density of dislocations in crystals may increase by several orders, while the displacement of the dislocation from one edge to another does not increase the length of the dislocation, and the emergence of the dislocation to the surface even reduces their overall density. The assumption of the existence in a crystal of Frank-Read dislocation sources and the experimental observation of the sources, solved the problem of dislocation multiplication, but it turned out that slip lines (steps formed at the emergence of dislocations to the surface) are significantly shorter in length than the size of strained crystalline samples. To solve this problem, it is usually assumed that shear-forming dislocation loops, emitted by the dislocation source, are stopped by strong dislocation barriers that arise due to the interaction of segments of expanding dislocation loops with reactive dislocations of non-coplanar glide systems, such as Lomer-Cottrell barriers. The formed barriers hinder further expansion of dislocation loops and, thereby, form the boundary of the shear zone. The length of slip lines observed on the surface of the strained crystal should correlate with the distance between the barriers.
Thus, there are problems needed to be solved: 1) to identify the types of potential barriers; 2) to determine conditions under which the barriers do not break under the influence of stress on dislocation segments in the glide plane; 3) to determine conditions under which the length of forming barriers is large enough to prevent bending of barriers by neighboring segments of the dislocation loop; 4) to estimate the size of the shear zone as the distance between barriers.

In [1-4] these problems were solved within the framework of certain assumptions, however a number of proposed solutions have significant drawbacks. The model of dislocation interactions, proposed by the authors, allows refining the parameters used in estimation of the shear zone size and, thus, to obtain more substantiated average sizes of the shear zone in FCC-crystals.

2. Various methods for estimating the shear zone size
The simplest method for estimating the shear zone size is processing of experimental data on the length of slip lines. The dependencies of the average length of slip lines \( L \) on the shear strain for copper single crystals with different orientation of the strain axis (Figure 1) were obtained in [5-7].

![Figure 1. The average slip line length [5-7]](image-url)

On the basis of these studies the empirical dependencies \( L \) on the degree of plastic strain have been proposed, such as \( L = \Lambda (a - a^*)^{-1} \), where \( \Lambda \) is the coefficient, \( a \) is the shear strain, \( a^* \) is the degree of shear strain in the beginning of the second stage of the strain [5, 1], or \( L = L_f + (L_i - L_f)e^{-KE} \), where \( L_i \) and \( L_f \) are the initial and the limiting length of a free path of the dislocation, \( k \) is the constant, \( \varepsilon \) is the strain degree [8]. These dependencies contain parameters that depend on strain conditions and cannot serve as the basis for mathematical modeling of plastic strain.

According to the known theoretical estimates, \( L \) is directly proportional to \( \rho^{-1/2} \) with coefficients varying within the limits of a single order, where \( \rho \) is the total dislocation density. Therefore, often the main parameters of models (the coefficient of the proportionality between \( L \) and the value \( \tau^{-1} \sim \rho^{-1/2} \)) are found based on the experimental data. It is known that this parameter depends on the crystal orientation, the orientation of moving dislocation segments, the temperature (\( L \) increases approximately by 3 times at a reduction in the temperature from 573 K up to 4,2 K [9]), the presence of impurities, and other factors. For screw segments in [100] – copper single crystals such dependence cannot be obtained from the experimental data [6], and in [111] – single crystals the dependence...
\( L = 50\rho^{-1/2} \) has been obtained (Figure 1). Furthermore, at the same value \( L \) the intensity of dislocation accumulation can vary significantly depending on the nature of dislocation distribution on the boundary of the shear zone and the geometry of the shear zone [2].

Thus, common to all materials and strain conditions the dependence \( L \) on the density of dislocations, stress, or strain has not yet been proposed.

Emergence of simplest dislocation models of plastic strain, in which the intensity of dislocation accumulation depends on the average size \( D \) of the shear zone diameter, has allowed estimating the shear zone size based on its connection \( \theta / \Delta a = 0.5\alpha G F \rho^{-1/2} D^{-1} \) with the hardening coefficient in the second stage of strain. However, for example, for [100] – single crystals it became impossible to accurately determine the end of the second stage of the experimental dependence. As a consequence, it is possible to obtain the values of the proportionality coefficient \( 0.5\alpha G F \rho^{-1} \) in the equality \( D = 0.5\alpha G F \rho^{-1} \) differing by the order of magnitude.

In [1, 3] the methods for theoretical estimation of the shear zone size have been proposed based on the assumption that the length of the dislocation path is determined by dislocations of non-coplanar slip systems. To form a barrier it is necessary for the stress of the interaction of reacting dislocations to be higher than the internal long-range stress \( \tau_2 \) in the secondary glide plane. Based on this condition, an effective capture radius \( r_c = 0.5\pi^{-1}\alpha G b \tau_2 \) is determined, where \( \alpha_c \) is the parameter considering the geometry of the dislocation distribution. The parameter \( \alpha_c \) has the value of an order \( 0.5 \), and, thus, the capture radius may vary within the limits of the same order of the magnitude, which leads to the same spread of the diameter size of the shear zone.

In [3] the expression \( D = B_2 G^{-1} b^{-1} \tau_2^{-1} \) for the diameter of the shear zone was obtained as follows. Assuming that the loop has a rectangular shape with the sides \( D \) and \( D_1 \), and the number of dislocations which interact with one of the sides during its path from the source at a distance of \( 0.5D \) equals to \( 0.25 D D \xi \rho \), where \( \xi \rho \) is the number of dislocations intersecting the unit area, \( \xi = \rho_f \rho_2^{-1} \approx 0.5 \) is the share of “forest” dislocations, \( \rho_f \) is the density of the “forest” dislocation. Barriers with the length \( D_1 \), capable to limit the length of the dislocation path, among all the reacting dislocations can form only \( \beta \) of “forest” dislocations which are inclined at a small angle to the glide plane of the loop. During the path of the glide dislocation at a distance of \( 0.5D \) such an event can occur only once, therefore \( 0.25 D D \xi \rho \beta = 1 \). Taken into account the fact that the reaction takes place under the condition \( \tau_2 \leq \alpha_c G b / 2\pi r_c \), we obtain the limiting value \( \phi_m = \text{arctg}(2r_1 D_1^{-1}) \approx \alpha_c G b \pi^{-2} D_1^{-1} \tau_2^{-1} \) of the inclination angle \( \phi \) of the forest dislocation to the junction line, at which the dislocation junction with the length \( D_1 \) can be formed. With a uniform distribution of values \( \phi \) the probability of formation of a compound with the length \( D_1 \) equals to \( \beta = \phi_\pi^{-1} = \alpha_c G b \pi^{-2} D_1^{-1} \tau_2^{-1} \).

As a result we obtain \( D = 4\pi^2 \tau_2 \alpha_c \beta^{-1} \xi^{-1} G^{-1} b^{-1} \rho^{-1} \). In the case of symmetric orientations of strain axes, when a slip is carried out under several equivalent systems, it can be assumed that \( \tau = \tau_2 \), then we obtain an expression for the diameter of the shear zone in the form \( D = B_2 G^{-1} b^{-1} \rho^{-1} \approx \alpha B_2 \rho^{-5/2} \), where \( B_2 = 4\pi^2 \alpha_c \beta^{-1} \xi^{-1} = 16\pi^2 \beta_\tau^{-1} \). Given that \( \beta_\tau = 0.14...0.25, \alpha \approx 0.25 \) we obtain \( B_2 \approx 1128, D \approx 282\rho^{-5/2} \), which is several times higher than the experimentally observed values.

The most accurate method for estimation of the shear zone size, in our opinion, can be based on the assumption that in the area \( S_A \), swept out by the dislocation loop, there are \( 4 \) dislocations at different
distances from the source that can form insurmountable barriers. Segments of the expanding dislocation loop are alternately stopped by these barriers, so that the final configuration of the shear zone boundary is a convex figure. Suppose $D$ is the share of dislocations that form barriers, then $S_D \beta \xi_D = 4$ is the number of barriers. If the value $D = S_D^{1/2}$ is taken as the average size of the shear zone, we obtain $D = 2(\beta D \beta \xi D)^{1/2}$. The value $\beta_D$ can be determined theoretically based on the model of dislocation interactions.

3. Estimation of parameters determining the diameter of the shear zone

To estimate the value $D$ it is necessary to determine parameters $\beta_r$ and $\beta_D$.

3.1. Estimation of the parameter $\beta_r$

As a result of dislocation reactions among dislocations of non-coplanar slip systems, dislocation junctions, which are obstacles for further motion of a slip dislocation, are formed at the intersection line of glide planes of reacting dislocations. To estimate the strength of dislocation junctions Schoeck and Frydman [10] proposed to determine the balance of a ternary dislocation node $E$ on the basis of the virtual displacement principle, according to which the displacement of the node $E$ (Figure 2) along the junction line is considered, and changes in the energy of dislocation segments are taken into account. In virtue of the task complexity a number [10] of simplifying assumptions have been introduced: 1) reacting dislocations intersect each other in the middle; 2) dislocation junction is motionless; 3) elastic interaction among dislocation segments is minor; 4) reacting dislocations are unextended; 5) forest dislocations are inflexible; 6) material is isotropic; 7) slip dislocations are screw or edgy only.

![Figure 2](image_url)

Figure 2. Examples of arbitrary intersections of reacting dislocations. The parameter $\gamma_s = QO : QP = 0.1 \div 0.9$ reflects the ratio of segment lengths of a slip dislocation. The parameter $\gamma_f = NO : NM = 0.1 \div 0.9$ reflects the ratio of segment lengths of forest dislocation. The point $O$ – is the intersection point of reacting dislocations. Intersections at different values of parameters are presented: a) $\gamma_s = 0.1$ and $\gamma_f = 0.1$; b) $\gamma_s = 0.4$ and $\gamma_f = 0.6$; c) $\gamma_s = 0.1$ and $\gamma_f = 0.5$.

This simplest model has been widely used in calculation of the strength of dislocation junctions in a number of papers by a group of authors with the weakening of certain simplifying assumptions. In particular, the authors of this paper have investigated the flexibility of forest dislocations and changes in the orientation of the axis of a slip dislocation with respect to the Burgers vector (change in the angle $\psi_1$).

As a result, for materials with a FCC structure the values of the parameter $\beta_r$ were obtained [11, 12], characterizing the probability of formation of a dislocation junction (Figure 2) for different orientations of the strain axis of a crystal. The value of the parameter $\beta_r$ was determined according to [13] using the relation $\beta_r = \rho_f \rho_s^{-1} = 36^{-1} \sum_{i=1}^{8} (1 - \cos \phi_i)$). The average value of the probability of formation of the junction $\beta_r$ strongly depends [11, 12] on the type of a slip dislocation (on the angle $\psi_1$). The maximum
value of the probability $\beta_r = 0.25$ corresponds to the 70\textsuperscript{th} slip dislocation, the minimum $\beta_r = 0.145$ corresponds to a screw dislocation, to an edge dislocation $\beta_r = 0.215$.

It should be noted that it was impossible to overcome some of the abovementioned simplifying assumptions within the framework of the Schoeck-Frydman model. Using the principle of virtual displacements [10, 13] it is impossible to directly determine the stress of a junction strain, to track changes in the geometry of the dislocation configuration under the influence of stress, as well as to overcome one of the strongest simplifying assumptions – the intersection of reacting dislocations in the middle, which is far from the actual intersection of dislocations in a crystal.

In this regard, the authors of this paper proposed a new model [14] enabling to describe the dislocation configuration, formed as a result of the reaction, in the real three-dimensional picture of the intersection of dislocations in non-coplanar slip systems.

3.2. Estimation of the parameter $\beta_D$

As part of the previously proposed model [14-16] by the authors of this paper, dislocation junctions at the intersection of arbitrary segments of reacting dislocations have been calculated. Intersections of reacting dislocations $QP$ and $NM$ (Figure 2) have been considered depending on the ratio of segment lengths $\gamma_f = NO : NM$ of the slip dislocation and the ratio of segment lengths of the forest dislocation ($O$ is the intersection point of dislocations). Length spectra of dislocation junctions have been calculated for the following values of parameters $\gamma_g = QO : QP = 0.1 ; 0.9$ and $\gamma_f = NO : NM = 0.1 ; 0.9$.

As a result of computational experiments, in the given model [14-16] the dynamics of changes in the whole dislocation system formed as a result of the reaction of dislocations of non-coplanar slip systems under the influence of the applied stress $\tau$, including its destruction, has been investigated. The change in the length of the dislocation junction has been studied directly under the influence of stress.

In the study of the destruction process of dislocation junctions the mechanism of formation of long dislocation junctions has been revealed [15, 16]. The essence of which consists in the following: under the applied stress a dislocation junction does not break but, on the contrary, its length increases. This occurs in the case when the position of dislocation nodes $E$ and $F$ begins to change under the influence of stress. At that, both nodes are moving along the junction line, but one of them, for example, the node $E$ is more mobile than the node $F$. As a result, under the influence of stress, the length of the dislocation junction increases exceeding the original length. It has been revealed that rather high stresses of nearly $100 \div 500$ MPa are needed for breaking of such junctions [16]. Long strong dislocation junctions are, practically, insurmountable barriers for motion of dislocations.

In this paper, a share of long insurmountable dislocation junctions, which were obtained at different intersections ($\gamma_g = 0.1 ; 0.9$ and $\gamma_f = 0.1 ; 0.9$) of reacting dislocations for all dislocation reactions implemented at orientation of the strain axis of the crystal [100], has been calculated. Each of these intersections has been considered for all types of slip reacting dislocations, from the screw orientation up to the edge orientation ($\psi_1 = 0^\circ \div 90^\circ$), in which the given reaction is implemented. Calculations have been performed for the whole range of angles of forest dislocations in the case of the initial inclination angle to the junction line $\varphi = 10^\circ$.

The lengths of junctions under the above listed conditions have been determined, and the quantity of long junctions has been obtained for different values of the dislocation density $\rho = 10^{10} \div 10^{14}$ m$^{-2}$ and for various dislocation reactions. According to the obtained results, a share of long junctions has been calculated for each implemented dislocation reaction. A share of strong (insurmountable) dislocation junctions from the total number of the obtained junctions has been determined [17].
Based on the obtained results, the probability of formation of a long strong dislocation junction for each value of the dislocation density has been determined using the total probability formula. From the analysis of the obtained results the average value of the parameter $\beta_D = 0.001$, characterizing the probability of occurrence of a long insurmountable dislocation junction in the case when the strain axis of the crystal is oriented towards [100], has been determined.

The presence of long strong dislocation barriers allowing blocking the motion of dislocations can be one of the mechanisms for determining the size of the shear zone.

4. Conclusion

The obtained estimates of the parameters $\beta_r$ and $\beta_D$ allow to obtain the value $2(\beta_r \beta_D)\frac{\xi}{\beta_D} \approx 80$ of the coefficient in the formula $D = 2(\beta_r \beta_D)\frac{\xi}{\beta_D}^{1/2}$ of the dependence of the shear zone diameter on the dislocation density. This value agrees well with a variety of experimental data on slip lines and the hardening coefficient in the second stage, which allows using this value in estimation of values characterizing the defect structure of the shear zone.

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