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# Peierls Stress for $[l l \overline{2 h}](h h l)$ Shear in the FCC Lattice 

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#### Abstract

Data on the orientation of bands of nonoctahedral shear in $\mathrm{Ni}_{3} \mathrm{Fe}$ single crystals upon compression in the [001] direction are discussed within the model of crystons-carriers of shear of the superdislocation type. The discussion is based on the model of the core of the cryston as a carrier of simple shear in a deformation band of finite thickness. A concept of the Peierls stress for a cryston, $\tau_{\text {P.cry }}$, is introduced, which is an analog of the Peierls stress $\tau_{\mathrm{P}}$ for a single dislocation. A formula is suggested for estimating $\tau_{\mathrm{P}, \text { cry }}$ in the case of shear on ( $h h l$ ) planes. The $\tau_{\text {P.cry }}$ dependence on the indices $h$ and $l$ is discussed. It is shown that, in the spectrum of observed orientations ( $h h l$ ), the greatest value of $\tau_{\text {P,cry }}$ corresponds to the orientation (23 2325 ) of the shearband boundary, which is the first to arise in the course of deformation (at $\varepsilon=9 \%$ ). Based on the assumption on the closeness of the stress $\tau$ that corresponds to the beginning of the formation of a band with (232325) boundaries to $\tau_{\text {P.cry }}$ for crystons that form this band, the width of the core of the partial dislocation that enters into the cryston core is estimated.


## INTRODUCTION

It was established previously $[1,2]$ that, upon symmetrical loading of $\mathrm{Ni}_{3} \mathrm{Fe}$ alloy crystals along the [001] axis, the sample is separated into local domains (fragments) in which, as a rule, two octahedral slip planes operate (different in different fragments). It is the presence of dislocations corresponding to two slip systems with intersecting octahedral planes that is the necessary condition for the onset of the formation of deformation bands of the nonoctahedral shear [3]. The main concepts of the model that describes the carriers of such a shear and some its geometrical features were developed in our previous works [4-6]. However, the problem of the nonoctahedral shear has one more important aspect. Since the movement of a cryston occurs in a periodic potential of a lattice, it is important to know the orientation dependence of the stress necessary to overcome the barrier without thermal activation. This stress is an analog of the Peierls stress $\tau_{\mathrm{p}}$ for a single dislocation; therefore, it is natural to use the designation $\tau_{\mathrm{P} \text {. cry }}$ for it. By the orientation dependence, we mean here the explicit dependence of $\tau_{\text {P.cry }}$ on the Miller indices $h, k$, and $l$ of the crystallographic planes ( $h k l$ ) on which the shear occurs. It is clear that a strong orientation dependence of $\tau_{\text {p.cry }}$ can lead to the existence of a limiting orientation $\left(h k l l_{0}\right.$ in the spectrum of possible boundaries of the shear bands which will separate some groups of orientations $(h k l)_{1}$ and $\left(h k l_{2}\right.$. Indeed, let inequalities $\left(\tau_{\text {P,cry }}\right)_{(h k)_{1}}>\left(\tau_{p_{\text {p cry }}}\right)_{(h k)_{1}}>\left(\tau_{\text {P,cry }}\right)_{(h k)_{2}}$ be fulfilled. Then, even if the condition for the generation of crystons $\tau>$ $\left(\tau_{\mathrm{cr}}\right)_{(h k)_{0}}$ is fulfilled (here, $\tau$ is the applied stress and $\tau_{\mathrm{cr}}$ is the critical stress required for the generation), the condition $\left(\tau_{\text {P.cry }}\right)_{\left(h k n_{0}\right.}>\tau$ will prevent the condition for cryston generation to be satisfied for the orientations
$(h k l)_{1}$, since it will block the process of bowing out of the working segment of the source of crystons. This latter condition also forbids the process of propagation of crystons on the $(h k l)_{1}$ planes, so that no shear bands with $(h k l)_{1}$ boundaries can be formed. Naturally, this inhibition does not extend on the $(h k l)_{2}$ orientations. A qualitative discussion of this problem and of the closely related problem of the structure of the cryston core are the main goals of this work.

For definiteness, below we will consider orientations ( $h h l$ ) of planar boundaries of shear bands that were observed in reality in the $\mathrm{Ni}_{3} \mathrm{Fe}$ alloy. Table 1 gives, along with the orientations ( $h h l$ ), the values of the angles $\varphi$ between the planes ( $h h l$ ) and the closest close-packed plane (111). We remember that, with increasing deformation, the change in the order of orientations in the observed discrete spectrum of orientations ( $h h l$ ) is characterized by a decrease of the $h / l$ ratio. When describing such bands, the plane (111) can be selected as a primary slip plane and the ( $11 \overline{1}$ ) plane can be selected as a secondary one. Since dislocations with [ $1 \overline{1} 0$ ] axes can exist in both these planes, we may choose (see, e.g., $[4,5]$ ) a model of a shear band in which the shear on the ( $h h l$ ) planes is realized by carriers with a "superposition" Burgers vector b consisting of $n$ Burgers vectors $\mathbf{b}_{1}$ and $m$ Burgers vector $\mathbf{b}_{2}$ of [1 $\overline{1} 0$ ] dislocations belonging to the main and conjugated slip systems, respectively ( $n \geq m$ ). For these shear carriers of the superdislocation type, a special term "cryston" was suggested in [4], in order to emphasize the crystallographic character of the shear (in the literature, the term "noncrystallographic shear" is used instead of the correct term "nonoctahedral shear").

Table 1. (hhl) boundaries of shear bands and the angles $\varphi$ between the ( $h \mathrm{hl}$ ) and (111) planes

| $(h h l)$ | $\left(\begin{array}{l}2323\end{array}\right)$ | $(111113)$ | $(557)$ | $(112)$ | $(113)$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\varphi, \operatorname{deg}$ | 2.28 | 4.62 | 9.45 | 19.47 | 29.50 |

Table 2. Values of the Schmid factor for the $[l l \overline{2 h}](h h l)$ shear

| $h / l$ | $1 / 1$ | $23 / 25$ | $11 / 13$ | $5 / 7$ | $1 / 2$ | $1 / 3$ | $1 / 5$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $M$ | 0.4714 | 0.4832 | 0.4920 | 0.4999 | 0.4714 | 0.3857 | 0.2619 |

Now, we make one more insignificant simplification: we assume that the Burgers vectors $\mathbf{b}_{1}$ and $\mathbf{b}_{2}$ are equal in magnitude and have a purely edge orientation with respect to the dislocation line [ $1 \overline{1} 0$ ], i.e.,

$$
\begin{equation*}
\mathbf{b}_{1}\left\|[11 \overline{2}], \mathbf{b}_{2}\right\|[112] . \tag{1}
\end{equation*}
$$

Requiring [3, 4] that the superposition Burgers vector

$$
\begin{equation*}
\mathbf{b} \| n \mathbf{b}_{1}+m \mathbf{b}_{2} \tag{2}
\end{equation*}
$$

lie on the $(h h l)$ plane, which is equivalent to the orthogonality of $\mathbf{b}$ with respect to the direction of the normal $\mathbf{N} \|[h h l]$, we obtain a simple relation between the index ratio $h / l$ and the numbers $n$ and $m$ that specify the contribution of the elementary shear carriers of the two octahedral slip systems at hand into the resultant carrier:

$$
\begin{equation*}
h / l=\frac{n-m}{n+m} . \tag{3}
\end{equation*}
$$

## SCHMID FACTOR FOR THE $[l l \overline{2 h}](h h l)$ SHEAR

Let us compare the resolved shear stresses $\tau_{\mathrm{r}}$ for shears on ( $h h l$ ) planes. We remember that $\tau_{\mathrm{r}}$ is proportional to the Schmid factor $M$

$$
\begin{equation*}
\tau_{\mathrm{r}} \sim M=\cos \varphi_{1} \cos \varphi_{2} \tag{4}
\end{equation*}
$$

where $\varphi_{1}$ and $\varphi_{2}$ are the angles between the applied stress and the directions of the normals $\mathbf{N}$ to the slip plane and the slip direction $\mathbf{b}$, respectively, in this plane. At $\mathbf{N}\|[h h l], \mathbf{b}\|[l l \overline{2 h}]$, the factor (4), both for the orientation of the compression axis along the [110] and [001] directions, reduces to the form

$$
\begin{equation*}
M=\frac{x}{x^{2}+1}, \quad x=\sqrt{2} h / l \tag{5}
\end{equation*}
$$

The values of the Schmid factor are given in Table 2, where, apart from the ( hhl ) orientations of shear bands that were observed in [001] single crystals of $\mathrm{Ni}_{3} \mathrm{Fe}$, orientations (115) and (111) are added for comparison.

It is seen that the Schmid factor is actually equal to the maximum possible value ( $M_{\max }=0.5$ ) for slip on (557) planes. For the (23 2325 ) and (11 11 13) planes, it is higher, and for the (112) plane, it coincides with the Schmid factor for the close-packed plane (slip on the (111) plane in this case occurs in the [11 $\overline{2}$ ] direction). The circumstance that the first of the orientations observed in the course of deformation, i.e., (23 2325 ), does not correspond to the maximum $M$ is not surprising, since, in the hierarchy of conditions necessary for crystons to be generated, the prior role belongs to the cryston composition, which traces the ratio of the fractions of dislocations of the two interacting slip systems (the ratio $n / m$ in (3)). In the course of deformation, the fraction of dislocations of the conjugated slip system increases; the parameter $n / m$ decreases; and, along with it, $h / l$ decreases as well.

## ESTIMATION OF THE PEIERLS STRESS FOR CRYSTON

We assume further that there is fulfilled a condition $\tau \geqq \tau_{\text {cr }} \geqq \tau_{\text {P.cry }}$, where

$$
\begin{equation*}
\tau_{\mathrm{cr}} \sim \frac{G b}{L} \tag{6}
\end{equation*}
$$

$b$ is the magnitude of the Burgers vector of the cryston, $G$ is the shear modulus, and $L$ is the length of the dislocation braid (a bundle of dislocations of the interacting slip systems) that plays the role of the operating segment of the generalized Frank-Read source [6]. Since the thickness of the braid is finite, it is obvious that the cryston represents a carrier with a deformation localized in a volume restricted along all three orthogonal directions. This circumstance should be taken into account when simulating the core of the cryston and, respectively, when estimating the magnitude of $\tau_{\mathrm{P}, \mathrm{cr}}$ -

At present, there exist efficient experimental methods of determining $\tau_{\mathrm{p}}$ for dislocations (see, e.g., [7]). For metals with an fcc structure (such as $\mathrm{Cu}, \mathrm{Al}, \mathrm{Au}$, $\mathrm{Ag}, \mathrm{Pb}$ ) in the case of octahedral slip, the reduced Peierls stress $\tau_{\mathrm{p}} / G$ was found to be less than $10^{-5}$ (note that in bcc metals the values of $\tau_{\mathrm{p}} / G$ are higher by two orders of magnitude). Theoretical (analytical) estimations of $\tau_{\mathrm{p}}$ are usually performed in the Peierls-Nabarro model [7, 8], according to which

$$
\begin{equation*}
\tau_{\mathrm{P}}=\frac{2 G}{1-v} \exp (-4 \pi \kappa), \quad \kappa=\frac{\zeta}{b} \tag{7}
\end{equation*}
$$

where $v$ is the Poisson ratio and $\zeta$ is the half-width of the dislocation in the slip plane.

It is natural to use, as a simple model of the cryston core, such a distribution of the displacement field in which the propagation of the field is accompanied by a simple shear deformation in the region of the motion of the shear-carrier core in the deformation band. If the shear deformation on the ( hhl ) plane is specified by the
magnitude of $\tan \Psi$, then such a shear can formally be considered to be a result of a cooperative motion of partial dislocations on each of the ( $h h l$ ) planes spaced by a distance

$$
\begin{equation*}
d_{h h l}=\frac{a}{\sqrt{2 h^{2}+l^{2}}} \tag{8}
\end{equation*}
$$

as this is shown schematically in Fig. 1, where $\tan \Psi=$ $\sqrt{2} / 4$. The sum of the Burgers vectors of partial dislocations should be equal to the magnitude of the superposition Burgers vector:

$$
\begin{equation*}
b=\sum_{j=1}^{N} b_{j[l l \overline{2} \bar{h}]} \tag{9}
\end{equation*}
$$

The number $N$ of terms in (9) is specified by the ratio

$$
\begin{equation*}
N=\frac{d}{d_{h h l}}=\frac{b}{\tan \Psi_{d h h l}} \tag{10}
\end{equation*}
$$

where $d$ is the dimension of the shear band in the direction $[h h l]$. We remind that the lattice translation vector in the $(h h l)$ plane along the $[l l \overline{2 h}]$ direction is equal to

$$
\begin{equation*}
\mathbf{b}=\frac{a}{2}[l l \overline{2 h}] \tag{11}
\end{equation*}
$$

where the integers $l$ and $h$ have no common factors. Then, from (11), (10), and (8). we have

$$
\begin{equation*}
N=\frac{2 h^{2}+l^{2}}{\sqrt{2} \tan \Psi} \tag{12}
\end{equation*}
$$

An estimate for the stress $\tau_{\text {P.cry }}$ for the above model of the shear-carrier core can be obtained by using the following approximation. Assuming that any (arbitrary) partial dislocation gives an equal contribution of the type (7) with a parameter

$$
\begin{equation*}
\kappa=\kappa_{i}=\frac{\zeta_{i}}{b_{i}} \tag{13}
\end{equation*}
$$

we find that

$$
\begin{align*}
& \left(\tau_{\text {P.cry }}\right)_{h h l}=\frac{2 G}{1-v} N \exp (-4 \pi \kappa) \\
& =\frac{\sqrt{2} G\left(l^{2}+2 h^{2}\right)}{(1-v) \tan \Psi} \exp (-4 \pi \kappa) \tag{14}
\end{align*}
$$

We emphasize that this estimate implies the stability of the cryston with a core structure shown in Fig. 1. Otherwise (decomposition into partial dislocations), the preexponential factor in (14) would not contain the factor $N$.

Now, we proceed with an analysis of the orientational dependence of $\tau_{\mathrm{P}, \text { cry }}$. Assuming that $\zeta_{i}$ is in a certain relation with $b_{i}$, we obtain from (14) a quadratic dependence of $\left(\tau_{\text {P.cry }}\right)_{h h l}$ on the Miller indices, which is


Fig. 1. Simple shear. Distribution of displacement fields.
specified by the preexponential factor. Then, for shear on planes with large values of $h$ and $l$, the magnitude of $\tau_{\mathrm{P}, \text { cry }}$ will substantially exceed the level of $10^{-5} \mathrm{G}$ typical of dislocations in the fcc metals and can even exceed $\left(\tau_{c r}\right)_{h h l}$ and thus suppress the generation of such shear carriers. Since the first orientation to be observed experimentally [2] in [001] $\mathrm{Ni}_{3} \mathrm{Fe}$ single crystals was an orientation with large indices $h=23$ and $l=25$, it is natural to assume that the inequality $\left(\tau_{\mathrm{cr}}\right)_{(232325)} \geq$ $\left(\tau_{\text {p.cry }}\right)_{(232325)}$ is still fulfilled for this orientation. As the $h / l$ ratio increases in the interval $1>h / l \geqslant 23 / 25$, we may expect a change in the sign of the inequality to the opposite: $\left(\tau_{\mathrm{P}, \mathrm{cry}}\right)_{\text {(hhl }}>\left(\tau_{\mathrm{cr}}\right)_{(h h l)}$. Then, for estimating the width of the core of a partial dislocation entering into the cryston, we may use the approximate equalities:

$$
\begin{equation*}
\tau \approx\left(\tau_{\mathrm{cr}}\right)_{(232325)} \approx\left(\tau_{\mathrm{P} . \mathrm{cry}}\right)_{(232325)} . \tag{15}
\end{equation*}
$$

On the basis of experimental data [9], we can choose a value $3.9 \times 10^{-3} G$ for $\left(\tau_{\text {cr }}\right)_{(232325)}$. Then, with allowance for (15), we find from (14) that $\kappa \approx 1.17$. It is obvious that, at $0 \leq h / l<23 / 25$, an inequality $\tau_{\text {cr }}>\tau_{\mathrm{P}, \text { cry }}$ should be fulfilled for $(h h l)$ planes and the Peierls stress should not play a significant part.

It is now expedient to discuss to which extent the estimates of $\tau_{\text {P.cry }}$ and $\zeta_{i}$ can change if we use a more consistent, than in the first variant of the PeierlsNabarro model, derivation of the formula for $\tau_{\mathrm{P}}$ which, in addition, also permits one to consider lattices other than simple cubic used in the original model. Note that the Peierls-Nabarro formula (7) is valid for sure for wide dislocations ( $\kappa \gg 1$ ); however, the lower boundary of $\kappa$ values for which (7) is valid is not clear. Joos and Duesbery [10] obtained a formula that is suitable for both wide and narrow dislocations:

$$
\begin{gather*}
\tau_{\mathrm{P}}(y)=-\frac{G b}{2 a} \sinh (2 \pi \kappa) \sin (2 \pi y)  \tag{16}\\
\times(\cosh 2 \pi \kappa-\cos 2 \pi y)^{-2}
\end{gather*}
$$



Fig. 2. Formal dislocation scheme of a carrier of simple shear.
where $a^{\prime}$ is the interplanar distance in the shear plane in the direction perpendicular to the dislocation axis; $\kappa=$ $\frac{\zeta}{a^{\prime}}$; and
$y=\frac{1}{2 \pi} \arccos \frac{1}{2}\left[-\cosh 2 \pi \kappa+\left(9+\sinh ^{2} 2 \pi \kappa\right)^{1 / 2}\right]$.
In the limiting case of narrow dislocations $(\kappa \ll 1)$, we have $\tau_{\mathrm{P}}=\frac{3 \sqrt{3}}{32 \pi^{2}} \frac{G b a^{\prime}}{\zeta^{2}}$ when $y$ tends to zero. For wide dislocations ( $\kappa \gg 1$ ), we obtain from (17) and (16) that $y=0.25$ and

$$
\begin{equation*}
\tau_{\mathrm{P}} \approx \frac{G b}{a^{\prime}} \exp (-2 \pi \kappa) \tag{18}
\end{equation*}
$$

It can easily be found that, at $\kappa=1$, we have $y \approx 0.2488$, which is close to 0.25 , and formula (18) is valid as before. For the limit of applicability of (18), we could assume the value of $\kappa$ at which the calculations of $\tau_{\mathrm{P}}$ by (18) and (16) would differ by no more than $10 \%$. A comparison of (18) and (7) exhibits a difference in both the preexponential factors and the exponents (see discussion in $[8,10])$. Taking into account that in the case of simple shear $[l l \overline{2 h}](h h l)$ we have $a^{\prime}=\frac{1}{\sqrt{2}} d_{h h l}$, expression (18) reduces to the form

$$
\begin{equation*}
\left(\tau_{\mathrm{P}}\right)_{h h l} \approx G\left[2 h^{2}+l^{2}\right] \exp (-2 \pi \kappa) \tag{19}
\end{equation*}
$$

where $\kappa$ includes the half-width $\zeta$ of the dislocation with a Burgers vector $\mathbf{b}$.

For the model of simple shear at $b_{i}=a^{\prime}$, we again obtain formula (19) with the help of (18); in this case, however, $\kappa$ includes the half-width $\zeta_{i}$ of the partial dislocation (at $\zeta_{i}$ on the order of $b_{i}=a^{\prime}$, we have $\kappa \sim 1$ ).

Thus, we again have a dependence on the indices $h$ and $l$, which is similar to (14). Requiring again that condition (15) be fulfilled and using (19), we find that $\kappa$ is approximately 2.06 at the same value of $\left(\tau_{\text {cr }}\right)_{(232325)}$. This latter estimate of $\kappa$, just as the previously estimated value, seems quite reasonable (the transverse size of the core of a partial dislocation is close to four interplanar spacings $a^{\prime}$ ).

Now, we proceed with an analysis of the effect of the exponential factor in (19) on the orientational dependence of $\tau_{\mathrm{P}, \text { cry }}$ Note first that the slip of quasi-planar crystons on ( $h h l$ ) planes with large (and almost coincident) values of $h$ and $l$ should be physically indistinguishable from slip on the octahedral plane (111). This means that $\left(\tau_{\mathrm{P}, \mathrm{cr})}\right)_{(h h n)}$ at the limiting transition $h \longrightarrow l \longrightarrow \infty, d \longrightarrow d_{h h l} \longrightarrow 0$ should be small (on the order of $\tau_{\mathrm{P}}$ for the octahedral slip of dislocations). Formula (19) apparently can describe such a limiting transition if we assume that $\zeta$ is of the order of the Burgers vector $b$ of the cryston, $a^{\prime} \ll b$, and $\kappa \sim\left(2 h^{2}+\right.$ $\left.l^{2}\right) \gg 1$. Then, the growing (quadratic in the indices $h$ and $l$ ) preexponential factor is efficiently truncated by the decreasing exponential factor (with an exponent which is also quadratic in the indices $h$ and $l$ ).

In reality, there is no need to perform the limiting transition $d_{h h l} \longrightarrow 0$, since there is a natural restriction from below on the magnitude of $d_{h h l}$, which permits one to establish to which extent the representation (actually used above) on the distinguishability of the nearest crystallographic planes ( $h h l$ ) is valid. To this end, we will use the uncertainty relation for the coordinate $\Delta x_{i}$ and momentum $\Delta p_{i}$ :

$$
\Delta x_{i} \Delta p_{i} \geq \frac{\hbar}{2}
$$

We assume that $\Delta x_{i} \sim d_{h h l}=\sqrt{2} d_{l l \overline{2 h}}$, and take into account that the minimum kinetic energy is $E_{k}=\frac{(\Delta p)^{2}}{2 m}$. Then, e.g., for the mass of an atom $m \sim 10^{-25} \mathrm{~kg}$, the energy $E_{k}$ for $\Delta x_{i} \approx d_{l l \overline{2 h}}$ corresponds to an absolute temperature of 410 K for the indices $h=95$ and $l=97$; i.e., the separate planes (959597) are physically indistinguishable already at room temperature. This conclusion appears to be even "more correct" for the planes with still larger indices. Taking into account that the (9595 97) plane makes an angle $\varphi \approx 0.565^{\circ}$ with the (111) plane, we may expect that slip on such planes (and on those that are more close to the close-packed planes) requires stresses that only insignificantly exceed $\left(\tau_{\mathrm{P}}\right)_{111}$. Note additionally that at a large (but fixed) value of the Burgers vector $b$ of the cryston, the limiting deformation of simple shear that has yet a physical meaning is described by the relation $\tan \Psi=$ $b / d_{h h l}$ and is localized in a layer of thickness $d_{h h l}$; i.e.,
the exponent in (19) for the case of a quasi-planar core of the cryston can be written as $-2 \pi \kappa \approx-2 \pi \tan \Psi$.

On the contrary, an increase in the transverse (with respect to the shear direction) size of the cryston core at a fixed Burgers vector of the cryston $\mathbf{b}$ should be accompanied by a decrease in the parameter $\kappa$ and, correspondingly, an increase in $\tau_{\text {p.cry }}$. The greatest value of $\tau_{\mathrm{P}, \text { cry }}$ may be expected for the motion of a dislocation wall (small $\tan \Psi$ ). Therefore, when estimating $\tau_{\text {p,cry }}$ for the deformation by simple shear in the interval $0<$ $\tan \Psi<b / d_{h h l}$, we can expect that the replacement of $\kappa$ by the factor $\kappa(\Psi)=(1+\tan \Psi) \zeta_{i} / d_{l \overline{2} \bar{h}}$ in the exponent in (19) would give a satisfactory interpolation.

## DISCUSSION

It is now interesting to compare the ratios of the Peierls stresses for shear carriers on ( $h h l$ ) planes. Assuming that the values of $\kappa$ only slightly change with changing $h$ and $l$ (i.e., fixing the values of $\tan \Psi$ ), neglecting the change in $G$, and using (19), we easily obtain

$$
\begin{gathered}
\left(\tau_{\mathrm{P}, \text { cry }}\right)_{(232325)} /\left(\tau_{\mathrm{P}, \mathrm{cry}}\right)_{(111113)} \approx 4.0 \\
\left(\tau_{\mathrm{P}, \text { cry }}\right)_{(111113)} /\left(\tau_{\mathrm{P} . \mathrm{cry}}\right)_{(557)} \approx 4.15 ; \\
\left(\tau_{\mathrm{P} . \mathrm{cry}}\right)_{(557)} /\left(\tau_{\mathrm{P} . \mathrm{cry}}\right)_{(113)} \approx 9 ;\left(\tau_{\mathrm{P}, \text { cry }}\right)_{(557)} /\left(\tau_{\mathrm{P} . \mathrm{cry}}\right)_{(112)} \approx 16.5 ; \\
\left(\tau_{\mathrm{P}, \mathrm{cry}}\right)_{(113)} /\left(\tau_{\mathrm{P}, \mathrm{cry}}\right)_{(112)} \approx 1.83
\end{gathered}
$$

For comparison, we remind that $\left(\tau_{\text {P.cry }}\right)_{(112)} /\left(\tau_{\text {P.cry }}\right)_{(111)} \approx 2$. We also remind that, in the case of $\left(\tau_{\mathrm{P} . \text { cry }}\right)_{(111)}$, the shear is performed along the [115 ] direction. It can be easily shown that $\left(\tau_{\text {P.cry }}\right)_{(111)}$ is 560 times less than $\left(\tau_{\text {P.cry }}\right)_{(232325)}$ and is $\sim 0.7 \times 10^{-5} G$. This value agrees well with the experimental value $\left(\tau_{\mathrm{P}}\right)_{(111)}<10^{-5}$ for dislocations given in [7]. This agreement is understandable. Indeed, the number of dislocations of the initial active slip systems whose interaction provides the generation of crystons decreases in the series of $\tau_{\mathrm{P}, \text { cry }}$ that are compared in the direction from $\left(\tau_{\text {P.cry }}\right)_{(232325)}$ to $\left(\tau_{\text {P,cry }}\right)_{(112)}$. For example, the shear on (112) planes can be produced by a cryston corresponding to only five initial dislocations ( $n / m=3 / 2$ ), and the transition to slip on (111) plane eliminates the participation of dislocations of the second slip system.

The above consideration shows that the strong orientation dependence of $\tau_{\mathrm{P}, \text { cry }}$ may become the factor that leads to the appearance of a forbidden range of ( hhl ) orientations of the boundaries of shear bands between (111) and (23 2325 ). This conclusion (based on the quadratic dependence of $\tau_{\mathrm{P}, \text { cry }}$ on the indices $h$ and $l$ ) indirectly indicates that the crystons that form the (23 2325 ) band have a core which substantially differs from a quasi-planar one. It is expedient to remind once more that the formation of a band with boundaries (23 23 25) is caused by the inclusion of dislocations of
the conjugated slip system into the process of generation of crystons.

One more note is relevant here. Prior to the appearance of shear bands with ( $h h l$ ) boundaries, a "coarsening" of the bands of octahedral shear is often observed. It is obvious from the above analysis that the process of coarsening of the bands can, in reality, be related to the generation of crystons with quasi-planar cores (i.e., low $\left.\tau_{\text {P,cry }}\right)$, which propagate on crystal planes (hhl) that make angles $\varphi$ of about $0.1^{\circ}$ with the octahedral plane. These orientations form a narrow range of quasi-continuous orientations close to (111). For such crystons, the relationship between the main and conjugated systems of dislocation slip obeys the inequality $n / m>10^{-}$ ${ }^{2}$. It cannot be ruled out that the boundary of the quasicontinuous range of orientations is specified by the constriction imposed by the uncertainty relation (see the end of the previous section), which determines the indices of the nearest planes ( $h h l$ ) that are physically indistinguishable. The formation of quasi-planar cryston cores for such slip plane systems seems to be quite natural.

The above explanation of the appearance of a range of forbidden orientations between (111) and (232325), naturally, is not the only possible one. An alternative explanation may reduce it to the problem of the realization of a generalized Frank-Read source capable of generating crystons from the range indicated; namely, (1) the number of dislocations composing the dislocation braid that represents the operating segment of the source can be limited; or (2) the length of the operating segment $L$ (bounded by the size of a crystal fragment or even of the whole sample) may be insufficient to satisfy conditions (6) necessary for generating crystons; and (3) the problem may be in the strength of the source. In spite of this, the suggested explanation has a more universal character, which is mainly related to the structure of the cryston core.

It should be noted that, when deriving the formulas used for the stresses $\tau_{\mathrm{P}}$ and $\tau_{\mathrm{P}, \text { cry }}$ we used the assumption of the smallness of atomic displacements in the direction perpendicular to the slip plane as compared to the displacement in the slip plane (it is assumed that the restoring forces connected with a bending of the bonds across the slip plane produce stresses only in the slip plane). It is clear that the correct allowance for the displacements in the [hhl] direction should increase the above-estimated value of $\left(\tau_{\mathrm{P}, \text { cry }}\right)_{h h l}$.

In the case of wide crystons with a small transverse (with respect to the shear direction) size of the core (quasi-planar core), $\tau_{\mathrm{p}}$ can be too small for slip on an arbitrary plane ( $h k l$ ) to be ensured because of the large magnitude of the parameter $\kappa$ which leads to the suppression of the preexponential factor (quadratic in the Miller indices) by the exponential factor.

## CONCLUSION

Estimates performed in terms of the dynamic approach show that, for the case of the simple shear in fcc crystals, the estimated magnitudes of $\tau_{\mathrm{p}, \text { cry }}$ and $\tau_{\mathrm{p}}$ do not contradict the experimental data. Moreover, the estimation indicates the possibility of generation and propagation of corresponding crystons in shear bands with a relatively wide range of orientations of ( hhl ) boundaries. As a nearest interesting problem to be solved, we suggest an analysis of the dependence of $\tau_{\mathrm{P}, \text { cry }}$ on the type of the configuration of the displacement field in the cryston, which differs from the configuration of the simple shear.

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