On the origin of microstructure self-similarity in severe plastic deformation

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(Dated: August 15, 2010)
Abstract

In a series of papers by D. Hughes, N. Hansen and their coauthors it was established that laminar microstructures developed in compression and rolling possess a surprising property: probability distribution of misorientations referred to the average misorientation is universal, i.e. slightly dependent on the material and the magnitude of plastic deformation. A similar fact was found for lamina spacings. This paper aims to derive these probability distributions from "first principles". As such two propositions are suggested: microstructures that are compatible with the prescribed physical and geometrical conditions are equiprobable, and the product misorientation × spacing cannot be smaller than some number. It turns out that the low bound for misorientation × spacing can be chosen in such a way that the experimental and theoretical curves coincide. The corresponding value of the low bound is in a nanoscale range.

Keywords: misorientation distribution, spacing distribution, severe plastic deformation, lamella microstructure

I. INTRODUCTION

One of the most remarkable experimental findings of recent years in material science was the discovery of self-similarity of microstructures in severe plastic deformations. It was made by Hughes et al. 1997a, 1997b and developed further in a series of publications by Hansen et al. 1999, Hansen 2001, Godfrey et al. 2000, 2004, 2005, Hughes et al. 1998, 2000, 2001, Liu et al. 1998. In these works the microstructure of cold rolled aluminum, copper and nickel was studied in case of large plastic deformation, up to a von Mises strain 6. In such highly deformed materials the microstructure is predominantly laminar (Fig. 1). The laminar microstructure exhibits the "turbulent" features: the misorientation angle of crystal lattices in neighboring laminae, \( \theta \), and lamina thickness, \( a \), are random. The probability density functions of \( a \) and \( \theta \) were found by working out the experimental data. It turned out that the random numbers, \( a \) and \( \theta \), after being scaled by their average values, \( \bar{a} \) and \( \bar{\theta} \), seem to have the universal probability distributions that are only slightly dependent on strains and materials tested. The experimental data are shown in Fig. 2. Note that the self-similarity of microstructures in Stage II plasticity, i.e. in the range of plastic deformation where the
flow stress depends linearly on strains, was envisioned long ago by D. Kuhlmann-Wilsdorf 1962. The experimental finding mentioned pertains mostly to stage III plasticity. In addition to lamellar structures, inside the laminae some foam-type microstructure develops. It was termed incidental dislocation boundaries (IDB). IDB also exhibit stochastic self-similarity.

Another important finding of the experimental research cited is a special role played by the product of average misorientation angle $\bar{\theta}$ and average spacing $\bar{a}$: it turned out to be practically constant in the range of von Mises strain $0.2 - 0.8$:

$$\bar{\theta}\bar{a} = 650b.$$  \hspace{1cm} (1)

Here $b$ is the interatomic distance.

This paper aims to test whether the experimental results described can be derived from the following "first principle": all microstructures that are compatible with the prescribed physical and geometrical conditions of an experiment are equiprobable. This proposition was used in the paper by Berdichevsky, 2008 to introduce and compute entropy of microstructure. The central point in applications of this proposition is a proper choice of the phase space and the constraints. We characterize each lamina by two parameters: its width, $a$, and the misorientation angle with respect to the original (undeformed) crystal, $\alpha$. The phase space
FIG. 2: Experimental data for probability density function of a) misorientation referenced to its average value $\bar{\theta}$, and b) lamina spacings referred to averaged spacings for various materials and strains (from Hughes et al. 1998).

is the space of all $a_1, a_2, \ldots$ and $a_1, a_2, \ldots$. Misorientations with respect to the original lattice, $\alpha$, and misorientations of two neighboring laminae, $\theta$, are different; we call them for brevity $\alpha$–misorientation and $\theta$–misorientation. We show that their averages, $\bar{\alpha}$ and $\bar{\theta}$, are linked as $\bar{\theta} = 2\bar{\alpha}$.

We complement the equiprobability of microstructures by another key assumption: there exists a "microstructure quantum" $\varkappa$ such that for each lamina of the microstructure

$$\alpha a \geq \varkappa.$$  \hspace{1cm} (2)

A motivation for (2) is discussed in Section 4. We find the value of $\varkappa$ by fitting the probability distribution of misorientations of our model to the experimental results (Fig. 11). The corresponding value of $\varkappa$ turns out to be in a nanoscale range:

$$\varkappa \approx 30b.$$  \hspace{1cm} (3)

For aluminum $\varkappa \approx 10nm$.

A possibility to obtain a qualitative (for spacings) and quantitative (for misorientations)
coincidence of experimental and theoretical probability distributions does not prove or disprove our basic assumption on equiprobability of microstructures because several other assumptions have been used as well. However, it indicates that equiprobability of microstructures is a reasonable starting point in studying the statistics of microstructures.

We begin with a description of a kinematical model for lamellar microstructures developed in compression (next Section). This kinematic scheme is meaningful only for small misorientation angles, therefore further consideration is constrained by the case of moderate strains \( \varepsilon \lesssim 1 \). Energy of interfaces is introduced in Section 3. The assumptions of the stochastic model are outlined in Section 4. The analytical treatment of the model is given in Section 5. In Section 6 we mention an interesting feature of microstructure energy, the inverse proportionality to squared lamina spacing.

II. KINEMATICS OF PLASTIC DEFORMATION: HOW A CRYSTAL ACCOMMODATES LARGE PLASTIC DEFORMATION BY DEVELOPMENT OF LAMELLAR MICROSTRUCTURE

At low/room temperatures plastic deformation of crystals is due mostly to nucleation and multiplication of dislocations. At low strain level the dislocations are distributed more or less randomly over the crystal body, sometimes forming tangles, clouds or bundles. At higher strains, the dislocations reorganize into more ordered structures. The geometry of these structures depends on the deformation mode, or, in general, on the load path. The dislocation structures developed in rolling and compression are described in detail in the papers by D. Hughes, N. Hansen and their coworkers cited above. The structures consist of two components: lamellar structures with a considerable misorientation on the interfaces\(^1\) and dislocation cell structures filling out each lamina. Dislocation cell structures are similar geometrically to closed cell foams. In what follows we focus on consideration of lamellar structures. The central goal of this Section is to establish a link between \( \alpha \)–misorientation and \( \theta \)–misorientation and motivate a choice of \( \alpha \)–misorientations as key kinematic para-

\(^1\) The interfaces were termed geometrically necessary boundaries (GNB). This name does not seem felicitous: all such boundaries are in fact, physically necessary, and we prefer to use the term interface.
meters of the microstructure. To this end we give a rough sketch of the way in which a lamellar microstructure can accommodate plastic deformations caused by compression. The reader who is interested only in the stochastic model and willing to take for granted the facts summarized at the end of Section, can skip this Section.

**lamellar microstructure.** Consider a piece of crystal compressed in $x-$direction (Fig. 3a). It is natural to assume that, in order to shrink in $x-$direction, two neighboring laminae deform as shown in Fig. 3b. In this Figure, thin lines are material lines of the crystal. We consider here a two-dimensional deformation. The shear deformation of two laminae in Fig. 3b can be accomplished by a set of dislocations shown in Fig. 4a. Indeed, the plastic strain $\varepsilon_{ij}^{(p)}$ associated with a dislocation is (see, e.g., Kunin 1983)

\[
\varepsilon_{ij}^{(p)} = \frac{1}{2} (b_in_j + b_jn_i) \delta (\Omega).
\]

Here $\Omega$ is the slip plane of the dislocation, $\delta (\Omega)$ the $\delta-$function of surface $\Omega$, $b_i$ and $n_i$ the components of Burgers vector and normal vector to $\Omega$, small Latin indices run through values 1, 2, 3. Emphasize that the dislocation is determined by the couple $\{b_i, n_i\}$: vector $b_i$ is equal to the jump of displacements on the two sides of the slip surface; the jump occurs when the initial state (the state of perfect lattice) is deformed to the current state; vector

![Figure 3](image-url)
FIG. 4: (a) A set of edge dislocations to accomplish the deformation in Fig. 3b; double lines are slip lines; (b) Symbolic picture illustrating the elongation of the layers by the two sets of dislocations in (a).

$n_i$ allows one to distinguish the two sides of the slip surface: if the two sides of $\Omega$, $\Omega_+$ and $\Omega_-$, are introduced in such a way that the normal vector is directed from $\Omega_-$ to $\Omega_+$, then Burgers vector is the difference of displacements on $\Omega_+$ and $\Omega_-$. Change of the sign of normal vector yields change of the sign of Burgers vector, while plastic strain tensor (4) remains the same. The symbol $\perp$ in Fig. 4a shows the edge dislocation location and at the same time indicates the direction of the extra half-plane. Vectors $\overrightarrow{b}$ and $\overrightarrow{n}$ in Fig. 4a correspond to the directions of extra half-planes shown. In a wider strip of Fig. 4a, $b_x < 0$, $n_x > 0$, therefore it follows from (4) that $\varepsilon^{(p)}_{xx} < 0$. In a narrower strip, $b_x > 0$, $n_x < 0$, and again $\varepsilon^{(p)}_{xx} < 0$, i.e. the widths of the two laminae decrease as a result of such plastic flow. The same can be concluded by noting that plastic strains (4) are incompressible: $\varepsilon^{(p)i} = 0$. The heights of the laminae grow as can be seen also from a symbolic picture in Fig. 4b. For convenience, in this Figure the deformation is shown as if there is one slip plane and the dislocations left the specimen: as follows from (4) plastic deformations in cases when dislocations left the body or just close to its boundary are practically the same. Due to incompressibility of plastic deformation, the widths of the laminae decrease.

We see that compression of the specimen can be accomplished by development of the set
of dislocations shown in Fig. 4a. Emphasize that both lamina thicknesses and distances between slip planes can vary, and the dislocation densities in the two laminae are, in general, different.

The issues on whether the material line $AB$ in Fig. 3 goes up or down, and how the crystal lattices rotate are more delicate. They require a more detailed discussion of kinematics of dislocation walls to which we proceed.

*Dislocation walls.* In this and the next two subsections we summarize the necessary relations of theory of dislocation walls; the derivation can be found in Berdichevsky 2010. Consider the dislocations that come to one side of an interface, the dislocation wall (Fig. 5). On the right of the dislocation wall the displacement field has jumps on the slip planes (or, in $2D$, slip lines) equal to Burgers vector. Far away from the wall on its right, the displacement gradient is practically zero between the slip lines. However, the displacement gradient averaged over an area on the right of the dislocation wall is not zero due to displacement jumps.
on the slip lines. The averaged displacement gradients on the right and on the left of the dislocation wall must coincide to avoid overlapping of the material points after deformation. The displacement distribution which develops on the left of the dislocation wall far away from the wall is shown for convenience at the vertical line CD. Let \( \vec{u}_R \) be the displacement vector at the distance \( R \) from the \( x \)-axis. The magnitude of this vector is equal to \( b \cdot (R/h) \), where \( h \) is the vertical distance between the slip lines; for large \( R \), \( R/h \) is the number of dislocations on the segment \( 0 \leq y \leq R \). At a point of the line \( CD \) with coordinate \( y = R \) \((R > 0)\) vector \( \vec{u}_R \) has the components

\[
\vec{u}_R = \left\{ \frac{R}{h} \cos \beta, \frac{R}{h} \sin \beta \right\}
\]

where \( \beta \) is the angle between the slip lines and the normal to the dislocation wall. The horizontal component of \( \vec{u}_R \) changes linearly along the vertical axis. It causes the rigid rotation of left half-plane. The rotation is symbolically shown in the insert of Fig. 5; in this insert, the rigid rotation of the whole body is fixed by the assumption that the part of the body on the right of dislocation wall does not rotate. For small angles of rotation, the angle of rotation, \( \alpha \), is

\[
\alpha = \frac{b}{h} \cos \beta.
\]  

(5)

Note that in this relation \( \cos \beta \) is finite. Smallness of \( \alpha \) is provided by a proviso that the distance between dislocations \( h \) is much larger than the interatomic distance \( b \).

The vertical component of \( \vec{u}_R \) also changes linearly along the vertical axis. This results in the vertical strain on the left of the dislocation wall,

\[
\varepsilon_{yy} = \frac{b}{h} \sin \beta.
\]

(6)

This is the only long range strain, all other strains and stresses decay exponentially from the wall on the distance of the order of \( h \). Clearly, such dislocation wall cannot exist without an external load, which produces the strain (6).

\[\text{In Fig. 5 the coordinates } \{x, y\} \text{ should be viewed as Lagrangian coordinates, i.e. the dislocation locations are the locations in the initial state. In the deformed state the dislocation wall is rotated. In calculation of stresses the difference between the dislocation positions in deformed and initial states is a nonlinear effect which can be neglected for small angles of rotation.}\]
We assume that no long range stresses develop in the microstructure. Therefore, there must be dislocations, which come to the other side of the interface. Consider a system of dislocations shown in Fig. 6. On the left of dislocation wall the stresses are zero. On the right of dislocation wall, the vertical component of displacement growth linearly in $y$ with the rate $b/h' \sin \beta'$. Therefore, on the right of dislocation wall it develops the vertical strain

$$\varepsilon_{yy} = \frac{b}{h'} \sin \beta'. \quad (7)$$

If we combine the dislocations of Figs. 5 and 6 into one wall, on the left and on the right of the wall the vertical stain $\varepsilon_{yy}$ is given by (6) and (7), respectively. This means that an extension load must be applied in vertical direction at infinity. If, however, the angles, $\beta$ and $\beta'$, and distances between the slip lines, $h$ and $h'$, are coordinated in such a way that

$$\frac{\sin \beta}{h} = \frac{\sin \beta'}{h'}, \quad (8)$$

then this load is the same on the right and on the left of the wall. Therefore, after release of this load, the stress state decays exponentially away from the wall. The relation (8) can be interpreted also as the condition of vanishing of the vertical component of the total Burgers vector on the interface. Such dislocation walls are "neutral": they do not produce long range stresses. Note that the long range stresses do develop, if the crystal is kinematically constrained at $y = \pm \infty$. In this case, a tension in the vertical direction appears. The tension is huge because $b/h$ could be of the order, say, $10^{-2}$. Therefore, they cause a secondary flow of dislocations which release the tension and makes the dislocation wall neutral (Jackson 1985, Brown 2002). In what follows, we assume that the crystal is traction-free at $y = \pm \infty$, while dislocation walls are neutral, and, thus, non-interacting.

**Crystal lattice misorientation angle.** Now we have to link the crystal misorientation and the plastic deformation. Crystal misorientation caused by a dislocation wall is introduced by an additional anzatz which is independent on the continuum model of dislocations. This anzatz postulates that a homogeneous dislocation flow does not change the orientation of a crystal. In Fig. 5, the orientation of the crystal in the initial state is shown by the sign #. In accordance with the anzatz, the orientation of the crystal lattice remains the same on the right of the dislocation wall. The left half-plane, if it is not constrained, must rotate for an angle $\alpha$. This causes the misorientation of crystal lattices in the deformed state as is seen
from the insert in Fig. 5. In this insert $AB$ is the position of the dislocation wall in the deformed state.

To see what is the misorientation caused by the dislocations that came to the other side of dislocation wall we draw the corresponding displacement field on the right of the dislocation wall (Fig. 6). It yields the misorientation shown in the insert of Fig. 6. Therefore the total misorientation caused by the superposition of the dislocation walls of Figs. 5 and 6 is the sum,

$$\theta = \alpha + \alpha'.$$  \hfill (9)

Apparently, (9) is meaningful only for small angles, when one does not distinguish $\theta$ and $\tan \theta$.

**Misorientations in lamellar structures.** Suppose that dislocations nucleated in each lamina remain in this lamina\(^3\). Moreover, let only one slip system operate in each lamina. Consider

\(^3\) Apparently, this is an approximation, but it seems reasonable on average because the free path of dislocations is about triple lamina spacing (Pantleon et al. 2001).
first just one lamina with a set of dislocations shown in Fig. 7a. On the two sides of the lamina the displacements are shown which develop away from the lamina to the right and to the left. This dislocation system produces an extension in the vertical direction as (6), but we ignore it because it will be released. The lines $ABCD, EFGH, BF$ and $CG$ are material lines. In the deformed state, according to the displacement field of Fig. 7a, the lines $BF$ and $CG$ are parallel; the lines $BC$ and $FG$ remain horizontal. The crystal on the left and on the right of the lamina is stress-free, and, therefore, moves as a rigid body. The resulting deformed state is shown in Fig. 7b. We see that the orientation of the crystal is the same on both sides of the lamina and different from the orientation in the lamina. For another slip

FIG. 7: Misorientation of crystal lattice caused by a homogeneous dislocation flow.
system shown in Fig. 7c, the corresponding deformed state is shown in Fig. 7d. Consider now two laminae, as shown in Fig. 8a. Combining Fig. 7b and Fig. 7d, and rotating Fig. 7d rigidly to make the line $DH$ the same on both Figures, we obtain the deformed state (Fig. 8b). If we vanish the region $CDHG$ by tending the line $CG$ to $DH$, we obtain the misorientation caused by two adjacent laminae (Fig. 8c). Adding further laminae we arrive at the deformed state depicted in Fig. 8d. In this Figure the lines shown are material lines.

Three outcomes of this kinematic picture are important for what follows. First, the misorientation in a lamina is determined only by the plastic distortion of this lamina and is not affected by plastic distortion of other laminae. In principle, for more complex geometries of dislocation networks long range influence may be observed. Second, the misorientation geometry can be characterized by a set of angles, $\alpha_1, ..., \alpha_N$, which describes the crystal rotation with respect to the original perfect crystal lattice. The angle for each lamina is determined by equation (5) while the misorientation at the interface by equation (9). Third, as follows from Fig. 8c, the symmetry axes follow the material lines $BC$ and $CM$. Fourth, there is no long range stresses in the dislocation network constructed. In other words, the interfaces do not interact if the distance between them is much greater than $h$.

Our kinematic scheme, as follows from Fig. 8d, yields the alternation of the misorientation angles. This feature supported by many experimental observations; one is reproduced in Fig. 9.

### III. INTERFACE ENERGY

For interface energy density per unit area we use formula which is a modification of the Read-Shockley formula (Read, Shockley 1950)

$$\gamma = \begin{cases} \gamma_m \theta / \theta_m & \theta \leq \theta_m \\ \gamma_m & \theta > \theta_m \end{cases}$$

where $\theta$ is the misorientation angle on the interface, $\gamma_m$ is a material constant, $\theta_m = 15^\circ$.

We are going to consider moderate strains, and, accordingly, small misorientation angles. Moreover, we would like to stay in the linear region of interface energy,

$$\gamma = \gamma_m \theta / \theta_m.$$  \hspace{1cm} (10)
Thus, we assume that $\theta \leq 15^\circ$. From (9), the angles $\alpha$ do not exceed $7.5^\circ$.

If a lamellar structure is characterized by a set of angles $\alpha_1, ..., \alpha_N$, and on $k$th interface $\theta_k = \alpha_{k-1} + \alpha_k$, then the total interface energy per unit area of the lamellar structure is the
FIG. 9: TEM images of 30% (a) and 50% (b) cold rolled aluminum (from Liu et al. 1998) show the alternation of misorientations along the microstructure.

\[ E = 2 \frac{\gamma_m}{\theta_m} (\alpha_1 + ... + \alpha_N). \]  

(11)

IV. A STOCHASTIC MODEL OF MICROSTRUCTURE

Consider the following highly idealized situation. A piece of crystal is clamped at one side, while the opposite side is compressed by a prescribed load (Fig. 10). We assume that

FIG. 10: Notation for laminar microstructure developed due to compression.
the plastic deformation is accommodated by the formation of a lamellar microstructure. The microstructure consists of $N$ laminae with the thicknesses $a_1, a_2, ..., a_N$. The plastic deformation of each lamina occurs due to nucleation and multiplication of dislocations. Dislocations sitting in a lamina cause the change of the crystal orientation of this lamina as compared to the orientation of the original crystal. The absolute value of the misorientation of $k$th layer is denoted by $\alpha_k$. As we have seen in Section 2, the absolute value of the crystal lattice misorientation is neighboring layers is equal to the sum,

$$\theta_k = \alpha_{k-1} + \alpha_k. \quad (12)$$

So, the microstructure is characterized by the set of $2N$ positive numbers, $a_1, a_2, ..., a_N$ and $\alpha_1, \alpha_2, ..., \alpha_N$. To describe the statistics of these numbers, we have to define the probability of elementary events. We use for that the following proposition: the microstructures with the same value of energy are equiprobable. It is assumed, of course, that the admissible parameters must satisfy the kinematic constraint: the sum of all lamina thicknesses must be equal to the length of the specimen, $L$,

$$a_1 + a_2 + ... + a_N = L. \quad (13)$$

The assumption of equal probability is, in a sense, a necessary one. It goes back to Laplace principle of insufficient reason: if we know nothing about the events, they should be claimed equiprobable. For, if they were not equiprobable, this means that we know something about these events.

Due to (11), the microstructures having the same energy per unit volume $U$, obey the constraint

$$\alpha_1 + ... + \alpha_N = N\bar{\alpha} \quad (14)$$

where $\bar{\alpha}$ relates to energy per unit volume as

$$\bar{\alpha} = \frac{UL\theta_m}{2\gamma_mN} = \frac{U\theta_m\bar{a}}{2\gamma_m}. \quad (15)$$

Here we introduced the average lamella spacing,

$$\bar{a} = \frac{L}{N}.$$
According to (14), the constant $\bar{\alpha}$ has the meaning of the average misorientation angle. It is convenient to write the geometrical constraint (13) in a form similar to (14):

$$a_1 + ... + a_N = N\bar{\alpha}.$$  \hspace{1em} (16)

Now we come to the key assumption of the model. In plastic deformation the values of $\alpha$ and $a$ fluctuate. However, it might be expected that the product $\alpha a$ cannot be very small. If $a$ is very small, i.e. one interface comes too close to another one, the interfaces interact, and one of them should disappear to reduce energy. Such process of a reduction of the number of interfaces when they become too close was observed indeed (Godfrey et al., 2000). The interface elimination process cannot be independent on misorientation. The larger misorientation, the more stable the structure is\(^4\). Therefore, we may expect that in the interface elimination process the determining parameter is not $a$, but $\alpha a$. So, we may expect that for observable microstructures the product misorientation $\times$ spacing has a low bound:

$$\alpha a \geq \varkappa.$$  \hspace{1em} (17)

Here $\varkappa$ is a parameter of dimension of length. The low bound $\varkappa$ has some similarity with Planck’s constant. Indeed, in the theory of heat radiation (the most detailed discussion was given in Planck 1913), the statistics of an ensemble of oscillators was based on an assumption that for one oscillator there is a minimum accessible volume of the phase space, Planck’s constant. Lamellar microstructure is an ensemble of laminae. As for an oscillator, the phase space of one lamina is two-dimensional. As in Planck’s theory we make small phase volume inaccessible. An important difference is that we do not introduce uncertainty $\varkappa$ for finite values of $\alpha$ and $a$. Of course, if we would do that, our results would not change. We call constant $\varkappa$ the microstructure quantum.

Perhaps, inequality (17) makes sense also on some pure technical ground. Laminae with small spacing, and, in general, grains with small sizes can be observed only if the size is large enough due to the restricted resolution of the instruments. Besides, the misorientation should be large enough to be observable. If only the product $\alpha a$ matters for observability, then (17) holds. In any way, in observations small $\alpha$ and small $a$ are lost, and this affects the experimental data, which we wish to describe.

\(^4\) This statement seems plausible for small misorientation angles, it is not clear if it holds for large angles.
Misorientation angles are also constrained from above. In 3D setting misorientation is an orthogonal transformation needed to make two crystal lattices coinciding. Orthogonal transformation is determined by the axis of rotation and the angle, $\theta$. This is the angle in Fig. 2a. The rotation angles are positive numbers not exceeding $2\pi$. For crystals possessing some symmetries, the misorientation angle defined as the minimum rotation angle needed to make two crystal lattices coinciding, can be less than $2\pi$. For example, for FCC lattices it does not exceed $62.8^\circ$. In the problem under consideration we admitted much stronger constraint assuming that $\theta$–misorientation angles are small. Thus, $\alpha$–misorientation angles are also small, and there is a number $\alpha_{\text{max}}$ such that

$$0 \leq \alpha \leq \alpha_{\text{max}}. \quad (18)$$

So, we arrive at the following mathematical problem: for given length of the specimen, $L$, energy per unit volume, $U$, and a number of laminae, $N$, find probability distribution of spacings $a$ and misorientations $\alpha$ that obey the constraints (14), (16) and (17). All points in the region

$$\bar{a}N \leq a_1 + \ldots + a_N \leq (\bar{a} + \Delta\bar{a}) N$$
$$\bar{\alpha}N \leq \alpha_1 + \ldots + \alpha_N \leq (\bar{\alpha} + \Delta\bar{\alpha}) N \quad (19)$$

are considered equiprobable. This means that the joint probability density of $\alpha_1, \ldots, \alpha_N, a_1, \ldots, a_N$ is

$$f(\alpha_1, \ldots, \alpha_N, a_1, \ldots, a_N) = C \delta(N\bar{a} - \alpha_1 - \ldots - \alpha_N) \delta(N\bar{a} - a_1 - \ldots - a_N) \theta(\alpha_1a_1 - \chi), \ldots, \theta(\alpha_Na_N - \chi) \quad (20)$$

where $\delta(x)$ and $\theta(x)$ are $\delta$–function and step function$^5$, respectively, $C$ the normalizing constant, $\alpha_i$’s change within the segment $[0, \alpha_{\text{max}}]$.

Due to symmetry with respect to transpositions of laminae, the joint probability density of misorientation and spacing of one lamina is

$$f(\alpha, a) = \int f(\alpha, \alpha_2, \ldots, \alpha_N, a, a_2, \ldots, a_N) da_2 \ldots da_N da. \quad (21)$$

$^5$ $\theta(x) = 1$ for $x \geq 0$, $\theta(x) = 0$ for $x < 0$. 

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Knowing \( f(\alpha, a) \), one can find probability distribution of misorientations, \( f(\alpha) \), and probability distribution of spacings, \( f(a) \), by integration. Probability distribution of misorientation at interface, \( f(\theta) \), is computed then from (12). We will find these distributions in thermodynamic limit when \( L \to \infty \) and \( N \to \infty \) while average spacing \( \bar{a} = L/N \) and energy per unit volume \( U \) are kept constant. Equivalently, one can keep \( \bar{a} \) and \( \bar{\alpha} \) constant, the latter is expressed in terms of \( U \) and \( \bar{a} \) from (15).

V. ENTROPY OF MICROSTRUCTURE AND PROBABILITY DISTRIBUTIONS

To find the asymptotics of the integral (21) as \( N \to \infty \) we proceed in the way which was suggested first by Lyapunov and has been used in similar problems, e.g., in Berdichevsky 1999, 2008, 2009. The key point is the computation of the phase volume,

\[
\Gamma_N(\bar{\alpha}, \bar{a}) = \int_{\alpha_1 + \ldots + \alpha_N \leq \bar{\alpha}^N} d\alpha_1 \ldots d\alpha_N da_1 \ldots da_N. \tag{22}
\]

It is convenient to deal with the dimensionless phase volume. Therefore, we introduce in the right hand side of (22) the factor \( \propto^{-N} \).

The phase volume can be written in terms of the step function as

\[
\Gamma_N(\bar{\alpha}, \bar{a}) = \int \theta(N\bar{\alpha} - \alpha_1 - \ldots - \alpha_N) \theta(N\bar{a} - a_1 - \ldots - a_N) \theta(\alpha_1 a_1 - \propto) \ldots \theta(\alpha_N a_N - \propto) d\alpha_1 \ldots d\alpha_N da_1 \ldots da_N / \propto^N. \tag{23}
\]

Since the derivative of the step function is \( \delta \)-function,

\[
\frac{\partial^2 \Gamma_N}{\partial \bar{\alpha} \partial \bar{a}} = N^2 \int \delta(N\bar{\alpha} - \alpha_1 - \ldots - \alpha_N) \delta(N\bar{a} - a_1 - \ldots - a_N) \theta(\alpha_1 a_1 - \propto) \ldots \theta(\alpha_N a_N - \propto) d\alpha_1 \ldots d\alpha_N da_1 \ldots da_N / \propto^N,
\]

and the normalizing constant in (20) can be expressed in terms of the phase volume:

\[
C = \left( \frac{\partial^2 \Gamma_N}{\partial \bar{\alpha} \partial \bar{a}} \right)^{-1} \propto^{-N}.
\]
We present the step function in terms of Laplace’s transform,
\[
\theta(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{xz} \frac{dz}{z},
\]
(24)
where integration is conducted in complex \(z\)-plane along the line \(\Re z = c > 0\). Substitution of (24) in (23) yields the integral:
\[
\Gamma_N(\bar{a}, \bar{a}) = \frac{1}{(2\pi i)^2} \int_{c-i\infty}^{c+i\infty} \int_{c'-i\infty}^{c'+i\infty} e^{NS(\bar{a}, a, z, \zeta)} \frac{dz}{z} \frac{d\zeta}{\zeta},
\]
(25)
\[
S(\bar{a}, a, z, \zeta) = z\bar{a} + \zeta a + \ln \int_{\alpha \geq x} e^{-z\alpha - \zeta a} da da.
\]
(25)

We seek the asymptotics of integral (25) as \(N \to \infty\). The asymptotics is determined by the points of minimum of \(S(\bar{a}, a, z, \zeta)\) over \(z, \zeta\) for real \(z\) and \(\zeta\). The minimum value of \(S\) has the meaning of entropy of microstructure (see Berdichevsky 2008).

It is convenient to make the change of variables \(z \to z/\bar{a}, \zeta \to \zeta/\bar{a}\), \(\alpha \to x : \alpha = x\bar{a}\), \(a \to y : a = y\bar{a}\). Variables \(x\) and \(y\) have the meaning of misorientation and spacings referred to their average values. Denote by \(m\) and \(k\) the numbers,
\[
m = \alpha_{\text{max}} / \bar{a}, \quad k = x / \bar{a}a.
\]
In new variables entropy takes the form
\[
S = z + \zeta + \ln \int_{\substack{0 \leq x \leq m \\\ \ 0 \leq y \leq k \\ \\ \ 0 \leq z \leq \zeta}} e^{-zx - \zeta y} dxdy - \ln k.
\]
So, entropy of microstructure is determined by a simple relation,
\[
S(m, k) = \Phi(m, k) - \ln k,
\]
(26)
\[
\Phi(m, k) = \min_{z, \zeta} [z + \zeta + \ln g(z, \zeta, m, k)].
\]
(27)
\[
g(z, \zeta, m, k) = \int_{\substack{0 \leq x \leq m \\ \ \ 0 \leq y \leq k \\ \ \ 0 \leq z \leq \zeta}} e^{-zx - \zeta y} dxdy.
\]
(28)

Denote the minimizers in (27) by \(\bar{z}\) and \(\bar{\zeta}\), the probability density function of misorientations and spacings by \(f(x)\) and \(f(y)\), respectively, and the probability density of misorientations
and spacings of one lamina by \( f(x, y) \). Let \( f(x, y; x', y') \) be the joint probability density of misorientations and spacings in two neighboring laminae. Then, as easy to see (Berdichevsky 1999, 2008, 2009), in the limit \( N \to \infty \) the parameters of the neighboring laminae become statistically independent, i.e.

\[
f(x, y; x', y') = f(x, y) f(x', y'),
\]

and

\[
f(x, y) = \text{const } e^{-\xi x - \zeta y}.
\]

Function \( f(x, y) \) is defined in the region

\[
0 \leq x \leq m, \quad xy \geq k.
\]

The normalizing constant in (30) is obviously equal to \( 1/g(z, \zeta, m, k) \).

Integrating (30) over \( y \) we obtain the probability density of misorientations.

\[
f(x) = e^{-\xi x} \int_{k/x}^{\infty} e^{-\zeta y} dy / g(z, \zeta, m, k) = e^{-\xi k / x - \zeta x} / \zeta g(z, \zeta, m, k).
\]

Integration (30) over \( x \) yields probability distribution of spacings

\[
f(y) = e^{-\zeta y} \int_{k/y}^{\infty} e^{-\xi x} dx = \left( e^{-\frac{k}{y}} - e^{-\zeta m} \right) e^{-\zeta y} / \zeta g(z, \zeta, m, k).
\]

Here \( y \geq k/m \). For \( y < k/m, f(y) = 0 \).

Since the misorientation at interface, \( \theta \), is the sum of misorientations in neighboring laminae, the average value of \( \theta, \bar{\theta} \), is equal to \( 2\bar{\alpha} \). For probability density of \( \theta^* = \theta / \bar{\theta} \) we have

\[
f(\theta^*) = M \delta \left( \theta^* - \frac{\alpha_1 + \alpha_2}{\bar{\theta}} \right) = \int_0^m \int_0^{m} \delta \left( \theta^* - \frac{x_1 + x_2}{2} \right) f(x_1) f(x_2) dx_1 dx_2
\]

\[
= 2 \int f(x_1) f(2\theta^* - x_1) dx_1.
\]

Here \( M \) stands for mathematical expectation, and \( f(x) \) is function (31). The limits of integration in the last integral of (33) are \([0, 2\theta^*] \) for \( \theta^* \leq m/2 \), and \([2\theta^* - m, m] \) for \( \theta^* > m/2 \).

Let us analyze the relations obtained. First of all, for \( m \) starting from the values 3 – 4, function \( g(z, \zeta, m, k) \) becomes practically independent on \( m \). From Fig. 2a, \( \theta / \bar{\theta} \leq 5; \)
apparently $\alpha/\bar{a}$ must be of the same order, and we can safely accept for $m = \alpha_{\text{max}}/\bar{a}$ the value 5 or greater. Thus, the only essential parameter is $k$. Second, probability densities are universal as long as $k = \varkappa/\bar{a}\bar{a}$ is universal, i.e. does not depend on materials and strains. Since $\varkappa$ was introduces as a universal constant, the issue is whether the product $\bar{a}\bar{a}$ is universal. This product is equal to $\bar{\theta}\bar{a}/2$, and its universality is an experimental fact: from (1)

$$\bar{a}\bar{a} = 325b.$$  

(34)

Function (33) fits well experimental data for $k = 0.1$ (Fig. 11). Note that in Figs. 11 and 12, we keep only experimental points that correspond moderate strains ($\varepsilon \lesssim 1$) and, thus, small average misorientations; for large misorientations the relation for the interface energy (10) which we have used is not correct. For $k = 0.1$ we get from (34) an estimate of $\varkappa = k\bar{a}\bar{a}$:

$$\varkappa \approx 30b.$$  

(35)

Probability distribution of spacings (32) for $k = 0.1$ deviates from experimental points (Fig. 12). It predicts larger number of small spacings. Perhaps, this is caused by the fact that a part of low angle interfaces, which is treated in our analysis as plane interfaces,
in experiment were crossed by IDB with the similar misorientation angles, and thus were treated as IDB and were not counted in spacing measurement for interfaces. Note also that the experimental points of Fig. 12 were obtained only in one experiment: this was compression of aluminum single crystal in [421]-direction at strains $\varepsilon = 0.2, 0.3$ and $0.6$; the writer is not aware of other experimental data for spacings at moderate strains.

VI. ENERGY OF MICROSTRUCTURE

An interesting outcome of our consideration is the formula for energy density of microstructure per unit volume

$$U = \frac{2\gamma_m}{k\theta_m} \cdot \frac{\kappa}{\bar{a}^2}. \quad (36)$$
Indeed, from definition of $\tilde{a}$ (15) we have

$$U = \frac{2\gamma_m}{\theta_m} \frac{\tilde{a}}{\bar{a}}. \quad (37)$$

Since $\tilde{a} = \frac{\kappa}{k}$, and $\kappa, k$ are some constants, we can rewrite (37) in the form (36).

Note the inverse proportionality of $U$ to $\bar{a}^2$. Such a dependence can appear only due to the presence in the theory of a parameter with the dimension of length, $\kappa$. Without such a parameter we would get from dimension reasoning the inverse proportionality of energy density to $\bar{a}$:

$$U = \text{dimensionless constant} \, \frac{\gamma_m}{\bar{a}}. \quad (38)$$

One can check that formula (36) corresponds to the values of energy density obtained by Godfrey et al. 2005. This serves as a circumferential evidence for feasibility to include in the theory a parameter with the dimension of length, the "microstructure quantum" $\kappa$.

The author thanks V. Segal and X. Wu for useful discussions.

**REFERENCES**


