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Rotation of crystal lattice induced by the development of dislocation slip in flat two-dimensional polycrystalline samples of aluminum with a "pancake" grain structure

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In this paper presented the results of the rotation of the crystal lattice of grains in flat samples of two-dimensional polycrystals of aluminum with a "pancake" grain structure "with an average grain size $d = 5 \div 15$ mm and initial dimensions of the working section 100 mm (length), 20 mm (width), 0.15 mm (thickness). Rotation of the grain crystal lattice occurs as a result of dislocation sliding during deformation of the samples by tension under active loading at a constant strain rate $\dot{\varepsilon} = 10^{-5}c^{-1}$ at room temperature. The features of such samples are following: there is only one layer of grains in the cross section and their sizes in the directions of the length and width of the sample significantly exceed the thickness of the sample; there is no constraint of the grain structure along the thickness of the sample. As a result, there is no constraint of plastic deformation in this direction. Experiment shows that slip deformation occurs predominantly in one slip system.

According to the well-known theoretical concepts of rotational plasticity, a model is proposed for the rotations of the crystal lattice of grains, which are caused by the action of one slip system. Calculations show that the trajectory of rotation of the tension axis on the plane of the stereographic projection is a circular arc, which is defined by the initial position of the tension axis. The equation for such a circles is obtained. Two cases of mutual arrangement of the tension axis, the normal to the sliding plane and the sliding direction are possible. If the initial crystallographic orientation of the grain is such that the tension axis lies in the plane of the sliding direction until it coincides with it. In this case, the tensile axis rotation traces cross point [101] as for a single crystal sample. In other case, when the directions of the tensile axis, sliding and normal to the sliding plane are not coplanar, then rotation trace does not pass through the point [101], but follows circular arc as mentioned earlier.

Comparison of the experimental data of the tensile axis rotation traces (based on the results of X-ray studies) with the calculated traces proposed by model (with one active slip system) shows their good agreement.

Keywords: flat two-dimensional aluminum polycrystals, active tensile plastic deformation, dislocation slip, grain crystal lattice rotation

Поворот кристалічної решітки внаслідок розвитку дислокаційного ковзання в плоских двовимірних полікристалічних зразках алюмінію з "млинцевою" зеренною структурою

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Наведено результати досліджень переорієнтації кристалічної решітки зерен у плоских зразках двовимірних полікристалів алюмінію з "млинцевою" зеренною структурою із середнім розміром зерен $d = 5 \div 15$ мм і початковими розмірами робочої частини 100 мм (довжина), 20 мм (ширина), 0.15 мм (товщина). Переорієнтація решітки зерен виникає внаслідок дислокаційного ковзання в процесі деформування зразків розтягуванням в умовах активного навантаження з постійною швидкістю деформації $\dot{\varepsilon} = 10^{-5}c^{-1}$ при кімнатній температурі. Специфікою таких зразків, у яких в поперечному перерізі є тільки один шар зерен і розміри зерен у напрямках довжини й ширини зразка істотно перевищують товщину зразка, є відсутність обмеженості зеренної структури по товщині зразка. Внаслідок цього відсутня утрудненість пластичної деформації в цьому напрямку. Згідно з експериментом деформація ковзанням здійснюється переважно в одній системі ковзання.

У межах відомих теоретичних уявлень про ротаційну пластичність запропоновано модель поворотів кристалічної решітки зерен, які спричиняє дія однієї системи ковзання. На підставі розрахунків показано, що траєкторією переорієнтації осі розтягування на площині стереографічної проекції є дуга кола, початкова точка якої відповідає початковій кристалографічній орієнтації зерна. Одержано рівняння такого кола. При цьому є можливими два випадки взаємного розташування осі розтягування, нормалі до площини ковзання й напрямку ковзання. Якщо вихідна кристалографічна орієнтація зерна є такою, що вісь розтягування розташована в площині напрямку ковзання й нормалі до площини ковзання, то поворот решітки зерна відбуватиметься так, що вісь розтягування наближатиметься до напрямку ковзання до збігу з ним.

У цьому випадку продовження траєкторії переорієнтації осі розтягування в спряженому стереографічному трикутнику потрапляє в точку [101] так само, як це відбувається для монокристалічного зразка. В іншому випадку, коли напрямки осі розтягування, ковзання й нормалі до площини ковзання є некомпланарними, продовження траєкторії переорієнтації в спряженому стереографічному трикутнику не потрапляє в точку [101], але прямує за згаданою вище дугою кола.

Порівняння експериментальних даних визначення траєкторії переорієнтації осі розтягування за результатами рентгенографічних досліджень із даними розрахунку на основі запропонованої моделі траєкторії переорієнтації осі розтягування внаслідок дії однієї системи ковзання свідчить про їхню добру узгодженість.

Ключові слова: плоскі двовимірні полікристали алюмінію, активна пластична деформація розтягуванням, дислокаційне ковзання, повороти кристалічної решітки зерен.

Разворот кристаллической решетки вследствие развития дислокационного скольжения в плоских двумерных поликристаллических образцах алюминия с "блинной" зеренной структурой Е.В. Фтёмов

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Представлены результаты исследований переориентации кристаллической решетки зерен в плоских образцах двумерных поликристаллов алюминия с "блинной" зеренной структурой" со средним размером зерен $d = 5 \div 15$ мм и исходными размерами рабочей части 100 мм (длина), 20 мм (ширина), 0.15 мм (толщина). Разворот решетки зерен возникает в результате дислокационного скольжения в процессе деформирования образцов растяжением в условиях активного нагружения с постоянной скоростью деформации $\dot{\varepsilon} = 10^{-5}c^{-1}$ при комнатной температуре. Спецификой таких образцов, у которых в поперечном сечении имеется только один слой зерен и размеры зерен в направлениях длины и ширины образца существенно превышают толщину образца, является отсутствие стесненности зеренной структуры по толщине образца. Вследствие этого отсутствует стесненность пластической деформации в этом направлении. Как показывает эксперимент, деформация скольжением осуществляется преимущественно в одной системе скольжения.

В рамках известных теоретических представлений о ротационной пластичности предложена модель поворотов кристаллической решетки зерен, которые вызывает действие одной системы скольжения. На основе расчетов показано, что траекторией переориентации оси растяжения на плоскости стереографической проекции является дуга окружности, начальная точка которой соответствует исходной кристаллографической ориентации зерна. Получено уравнение такой окружности. При этом возможны два случая взаимного расположения оси растяжения, нормали к плоскости скольжения и направления скольжения. Если исходная кристаллографическая ориентация зерна такова, что ось растяжения лежит в плоскости направления скольжения и нормали к плоскости скольжения, то поворот решетки зерна будет происходить так, что ось растяжения приближается к направлению скольжения до совпадения с ним. В этом случае продолжение траектории вращения оси растяжения в сопряженном стереографическом треугольнике проходит через точку [101] так же, как это происходит для монокристаллического образца. В другом случае, когда направления оси растяжения, скольжения и нормали к плоскости скольжение траектории в сопряжения и нормали к плоекости скольжения оси растяжения, скольжения и нормали к плоскости скольжения с ним. В этом случае продолжение траектории вращения оси растяжения не компланарны, продолжение траектории переориентации в сопряжения, скольжения и нормали к плоскости скольжения оси растяжения, скольжения и нормали к плоскости скольжения оси растяжения, скольжения и нормали к плоскости скольжения оси растяжения, скольжения и нормали к плоекости скольжения оси растяжения, скольжения и нормали к плоскости скольжения в сопряжение траектории вреисталлическом треугольнике проходит через точку [101], но идет по упомянутой выше дуге окружности.

Сравнение экспериментальных данных определения траектории поворота оси растяжения по результатам рентгенографических исследований с данными расчета на основе предложенной модели траектории поворота оси растяжения вследствие действия одной системы скольжения свидетельствует об их хорошем соответствии.

Ключевые слова: плоские двумерные поликристаллы алюминия, активная пластическая деформация растяжением, дислокационное скольжение, повороты кристаллической решетки зерен.

1. Introduction

Plastic deformation of macroscopic single crystals and polycrystals of metals has been studied in detail for a long time [1, 2]. Recently, attention has been focused on the analysis of strain hardening of micro- and nanocrystalline samples, including those with a transverse size in the micro- and nanoscale, as a promising materials for miniaturization of devices in the medical industry, microelectronic industry and nanotechnology, etc. [3 - 6]. At the same time, in practice, thin films, foils and plates are widely used, which have one to several layers of grains are located in the thickness of a polycrystalline material.

In this regard, it is important to study the mechanical properties of flat two-dimensional polycrystalline samples with the so-called "pancake" grain structure or close to it, when there is only one layer of grains in the cross section of the sample, and the grain sizes in the directions of the length and width of the sample significantly exceed the thickness of the sample [3, 6-10].

For coarse-grained flat two-dimensional polycrystalline samples with a "pancake" grain structure, one of the important factors determining their mechanical behavior is the crystallographic orientation of the grains. During the process of plastic deformation, the shape and size of the grains, as well as their crystallographic orientation are changing [10 - 17]. This work is devoted to the study of grain crystal lattice orientation changes of aluminum samples due to the development of dislocation slip under conditions of uniaxial tensile deformation.

2. Experimental procedure 2.1. Specimen preparation

To analyze the lattice rotations during plastic deformation, large grained specimens of pure aluminum (99.96 %) were used. Samples were taken from rolled polycrystalline aluminum foil 0.15 mm thick. Samples with dimensions 100 mm long, 20 mm wide, and 0.15 mm thick were cut from foil in the rolling direction. In order to relieve internal stresses caused by foil rolling, the samples were annealed for 2 hours at T = 400 °C. Then samples were deformed by uniaxial tension to $\varepsilon = 3\%$ and annealed at temperatures T = 300 °C (2 hours) and T = 630 °C (2 hours), which made it possible to obtain samples with an average grain size $\overline{d} = 5 \div 15$ mm, so that only one layer of grains (two-dimensional polycrystal) was placed in the cross section of the sample, and a "pancake" grain structure was formed, in which the grain sizes in the directions of length and width of the sample significantly exceeded the thickness of the sample.

2.2. Specimen surface and grain structure

The grain structure on the surface of the samples was revealed by chemical etching using an etchant of the following composition: 30 ml of HCl, 20 ml of HNO₃, 5 ml of HF, 30 ml of H₂O (etching time is 10 s).

The crystallographic orientation of grains in twodimensional aluminum polycrystals before and after deformation was determined by the direct Laue method. To study the deformation relief on the surface of grains of twodimensional aluminum polycrystals, an MIM-8 optical microscope and a Jeol JSM-840 scanning electron microscope were used.

2.3. Tensile testing

As it is known, the loading method has a significant effect on the nature of the plastic deformation of the metal. Plastic deformation of a polycrystal under load is provided by two mechanisms - translational and rotational [13]. The second one is caused by the appearance of a field of turning moments in a deformable solid. Depending on the type of loading, various methods of relaxation of this field are implemented. Experiments on active tensile loading are fundamental, since they make it possible to involve practically all the mechanisms of relaxation of the rotational moment field due to a continuous increase in the external load with a change in the rate and degree of deformation over a wide range [13]. Therefore, in this work, mechanical tests of two-dimensional aluminum polycrystals were carried out by tension under conditions of active loading. The samples were tested on air with a constant strain rate $\dot{\varepsilon} = 10^{-5} \text{ s}^{-1}$ and temperature T = 293K until the failure.

3. Dislocation slip and rotations of the grain lattice 3.1. Model

During the movement of individual dislocations, the translation of the nodes of the crystal lattice occurs, but the direction of the crystallographic axes remains unchanged. The emerging shears of the layers of the crystalline material can be well illustrated by the model of sliding plates (Fig. 1) In this case, the sample axis AB, which coincides with the tensile axis before the onset of deformation, changes its position in space (Fig. 1b) [1, 17]. Thus, the free movement of dislocations along the crystal causes the shape change and rotation of the AB axis of the sample, without changing the crystallographic orientation (rotation with an invariant lattice) [12, 13]. However, in the presence of rigid grips of the tensile testing machine, which can only move along the tensile axis, such change in the direction of the AB axis, i.e. rotation with an invariant lattice (Fig. 1b) is impossible. Under conditions of active loading, the sample axis must always coincide with the tensile axis (Fig. 1c). In a single-crystal sample, the fulfillment of this requirement leads to a rotation of its crystal lattice (Fig. 1c), while the direction of sliding turns to the tensile axis, tending to coincide with it [1, 11, 17].





When moving from a single-crystal sample to a polycrystalline one, the nature of plastic deformation becomes much more complicated. The requirement to preserve the continuity of the material makes it impossible to rotate with an invariant lattice of a grain in a polycrystal. For the selected grain, the surrounding grains at first approximation represent a rigid matrix. Grain boundaries are effective barriers to moving dislocations. They cause constraint of plastic deformation starting from the early stages of its development. As a result, reactive forces arise that cause plastic rotation of the selected grain relative to the surrounding rigid matrix [12, 13]. This causes a change in the crystallographic orientation of the grain. A quantitative description of this rotation is based on calculations of shear deformation in active slip systems [11 - 14]:

Rotation of crystal lattice induced by the development of dislocation slip in flat two-dimensional polycrystalline samples of aluminum with a "pancake" grain structure

$$\Delta \vec{\boldsymbol{\omega}} = -\frac{1}{2} \sum_{p} \Delta \gamma_{p} \left[\vec{\boldsymbol{n}}_{p}, \vec{\boldsymbol{t}}_{p} \right], \tag{1}$$

where $\Delta \bar{\omega}$ is rotation leading to plastic rotation of the crystal lattice; $\Delta \gamma_p$, \vec{n}_p and \vec{t}_p are the increment of the shear deformation, the normal to the slip plane, and the unit vector in the shear direction for the p-th active slip system respectively.

The aim of this work is to study this type of rotation in two-dimensional aluminum polycrystals with a "pancake" grain structure. The feature of such objects is that there is no constraint of plastic deformation along the thickness of the sample [9, 10], as a result, dislocation slip in grains occurs practically only in the primary slip system, as observed by the experimental data (Fig. 2).



Fig. 2. Images of the surface of grains of deformed specimens with traces of dislocation slip, obtained using an MIM-8 optical microscope (a) and a Jeol JSM-840 electron microscope (b).

Based on equation (1) the following expression can be written:

 $\vec{\boldsymbol{\omega}} \| \begin{bmatrix} \vec{\boldsymbol{t}} & \vec{\boldsymbol{n}} \end{bmatrix}, \qquad (2)$

i. e. the axis of rotation of the crystal lattice of the grain is perpendicular to the plane lying on the unit vectors of the normal to the slip plane \vec{n} and the direction of slip \vec{t} of the primary slip system. From (2) it follows that during the process of deformation the axis of rotation $\vec{\omega}$ does not change its direction, and the vectors \vec{n} and \vec{t} rotate in the plane perpendicular to $\vec{\omega}$. That means means the angle between the axis of rotation $\vec{\omega}$ and the tensile axis $\vec{\sigma}$ remains constant. We will examine two coordinate systems: laboratory (one of the axes of which is the axis of tensile $\bar{\sigma}$), and crystallographic (axes of which are the crystallographic directions in the grain of the polycrystal). The rotation of the crystal lattice during the process of plastic deformation means the rotation of the crystallographic coordinate system relative to the laboratory one. In the crystallographic coordinate system, a constant angle between $\vec{\omega}$ and $\vec{\sigma}$ means that during the process of grain rotation, the tensile axis precesses around the direction of the rotation axis (Fig. 3).

If the initial crystallographic orientation of the grain is such that the tensile axis $\bar{\sigma}$ lies in the plane of the vectors \vec{n} and \vec{t} , then the grain will rotate so that the direction $\vec{\sigma}$ moves towards \vec{t} and angle between them tends to zero. In this case, trace of $\vec{\sigma}$ on the stereographic projection goes to pole [101] as for a single-crystal sample [1, 10, 11]. Another case is when three unit vectors \vec{n} , \vec{t} and $\vec{\sigma}$ are not coplanar, i.e. when the angle between $\bar{\omega}$ and $\bar{\sigma}$ is not a right angle (Fig. 3). Calculation shows that trace of the $\vec{\sigma}$ axis on the stereographic projection does not pass through the [101]. Indeed, if we choose $(11\overline{1})[101]$ as the primary slip system, then in the crystallographic coordinate system of the grain, the unit vector of the rotation axis is defined as $\overline{\omega} = [1, -2, -1] / \sqrt{6}$. The precession of the end of the unit vector $\mathbf{\bar{\sigma}}$ means that it is moving on a circle (Fig. 3), the equation of which on the stereographic projection can be written as:

$$\left(\boldsymbol{u}-\boldsymbol{u}_{0}\right)^{2}+\left(\boldsymbol{v}-\boldsymbol{v}_{0}\right)^{2}=\boldsymbol{R}^{2},$$
(3)

where $\boldsymbol{u}, \boldsymbol{v}$ are the coordinates of a point on a circle in the stereographic projection plane, $\boldsymbol{u}_0, \boldsymbol{v}_0$ are coordinates of the center and \boldsymbol{R} is the radius. For the primary system: $\boldsymbol{u}_0 = -2/(1+\sqrt{6}(\boldsymbol{\bar{\omega}},\boldsymbol{\bar{\sigma}})), \qquad \boldsymbol{v}_0 = -1/(1+\sqrt{6}(\boldsymbol{\bar{\omega}},\boldsymbol{\bar{\sigma}})),$ $\boldsymbol{R} = \sqrt{(1-(\boldsymbol{\bar{\omega}},\boldsymbol{\bar{\sigma}})^2)/(1/\sqrt{6}+(\boldsymbol{\bar{\omega}},\boldsymbol{\bar{\sigma}}))^2}.$



Fig. 3. Scheme of the trace of the tensile axis $\mathbf{\bar{\sigma}}$ on the sphere of stereographic projection during rotation of the grain crystal lattice during deformation ($\mathbf{\bar{n}}$, $\mathbf{\bar{t}}$, $\mathbf{\bar{\omega}}$, $\mathbf{\bar{\sigma}}$ are unit vectors).

Fig. 4 shows the traces of the tensile axis $\vec{\sigma}$ on the stereographic projection during the rotation of the grain crystal lattice during deformation in case when primary slip system $(11\overline{1})[101]$ is active. These traces should be observed in the main stereographic triangle, since the slip system $(11\overline{1})[101]$ has the maximum Schmid factor within this triangle.



Fig. 4. Circles on the stereographic projection corresponding to equation (3).

When the projection of the tensile axis $\bar{\sigma}$ reaches the boundary of the standard and its conjugate stereographic triangles, the conjugate slip system should be activated and

double slip should occur [1]. Therefore, it is of interest to construct the traces of the tensile axis for a conjugate slip system from a conjugate stereographic triangle. The problem is solved similarly as for a standard triangle. The corresponding traces are shown in Fig. 5.



Fig. 5. Traces of the tensile axis $\bar{\sigma}$ on the stereographic projection during the rotation of the grain crystal lattice during the deformation for the cases of action of only the primary (standard triangle) and conjugate (conjugate triangle) slip systems.

As can be seen from Fig. 4 and 5, traces of the tensile axis for primary slip system $(11\bar{1})[101]$ depend on the initial crystallographic orientation of the grain and are not pass through [101], that fundamentally distinguish the evolution of the rotation of a polycrystal grain from the rotation of a single-crystal sample. As noted, an exceptional case is when the vectors \vec{n} , \vec{t} and $\vec{\sigma}$ are coplanar. Then the traces of the tensile axis tends exactly to the [101].

3.2. Experimental results and discussion

To verify proposed model, calculated traces of the tensile axis rotation based on Eq. (3) must be compared with the experimental data. It should be noted that the validity of the assumption about the dominant effect of the primary slip system is confirmed by the results of studying the surface of deformed samples by optical and electron microscopy. On fig. Figure 2 shown images of the deformation relief of the grain surface, illustrating the fact that, in most cases, dislocation slip in grains of two-dimensional polycrystalline aluminum foils with a "pancake" grain structure under active tension at room temperature occurs mainly in one primary slip system. The images of the microstructure clearly show traces of sliding only for the primary system within grains (Fig. 2a) and at

Вісник ХНУ імені В.Н. Каразіна, серія «Фізика», вип. 34, 2021

the boundary of two grains (Fig. 2b). Vertical lines parallel to the tensile axis $\vec{\sigma}$ are residual traces of foil rolling (samples were cut parallel to the rolling direction during preparation). Such mechanical behavior of two-

dimensional polycrystals is presumably can be related to absence of constraint in the grain structure (there is only one layer of grains), as same holds for plastic deformation over the thickness of the sample.



Fig. 6. Orientation of the tensile axis before and after deformation in grains of two-dimensional polycrystalline aluminum foils with a "pancake" grain structure, determined from the data of X-ray studies, and model traces of rotation of the tensile axis, calculated assuming the action of the primary slip system only.

To compare the calculated traces of the rotation of the tensile axis with the experimental data, the crystallographic orientation of grains of two-dimensional polycrystalline aluminum foils with a "pancake" grain structure was determined by X-ray before and after deformation. The results are shown in Fig. 6. For grains in which tensile axis $\vec{\sigma}$ before deformation lies in the plane based on the vectors of the normal to the slip plane \vec{n} and the slip direction \vec{t} , the trace of the rotation of the tensile axis tends to [101] (grain 2 in sample 6 in Fig.6f) as for a single crystal sample. For grains in which before deformation the vectors \vec{n} , \vec{t} and $\vec{\sigma}$ are not coplanar, the rotation trace does not intersect [101], but moves along the circular arc described by equation (3). Thus, the rotation of the crystal lattice of grains in a polycrystal is fundamentally different from the rotation of a single-crystal sample, for which the trace of rotation of the tensile axis must always cross [101]. Comparison of the experimental traces of rotation of the tensile axis (according to the results of X-ray diffraction determination of the crystallographic orientation of grains before and after deformation) with the calculated traces of the rotation of the tensile axis due to the action of the primary slip system indicates their good agreement. It should be noted that, according to [4, 18], the operating slip system in thin crystals and foils might be a system with not the highest Schmid factor. Experiments show that the active system is the one for which the path length of edge dislocations to the sample surface is minimal, which provides the smallest dislocation hardening. In our samples, the active slip system within the grain was either a system with a maximum value of the Schmid factor, or a system with a value close to it. If the active slip system is not the primary system (the one with the maximum Schmid factor), then this does not affect the nature of the traces of the tensile axis rotation, in the sense that the traces are still determined by Eq. (3). In this case, the axis of rotation $\vec{\omega}$ determined according to (2), the traces (circular arcs) of the axis rotation along with the corresponding coefficients of equation (3) will be different than for the primary slip system. However, this does not fundamentally change anything in our model.

It should be noted that for some grains, for example, on Fig. 6 (grain 2 in sample 1, grain 3 in sample 3, grain 2 in sample 4, grain 5 in sample 5), the projection of the tensile axis during the process of rotation "overshoots" into the conjugate stereographic triangle and moves in the direction of the circular arc determined by the equation (3), but deviating from the calculated trace. The reason for this seems to be that the secondary slip system is activated. In this case, for the theoretical calculation of the rotation traces, it is necessary to use relation (1), which takes into account the contribution of all operating slip systems. However, the fact that, during the process of rotation, the projection of the tenstion axis is not stay at the boundary of the standard and conjugate stereographic triangles, but "overshoots" into the second triangle, indicates the dominance of the primary slip system. Differences in the degree of rotation of different grains are caused by differences in the local deformation of these grains. With an increase in the degree of local deformation, the angle of rotation of the crystal lattice also increases.

4. Conclusions

1. A model for the rotation of the FCC lattice of grains of a two-dimensional polycrystals with a "pancake" grain structure due to the development of dislocation slip in the primary slip system upon deformation under active tension is proposed. An equation for the rotation traces of the tensile axis on the stereographic projection during the process of deformation is derived.

2. Modeling of the tensile axis rotation traces shows that, depending on the initial crystallographic orientation of the polycrystal grain, two cases of rotation are possible. If the tensile axis before deformation lies in the plane containing normal to the slip plane and the slip direction, then the trace of rotation passes through [101] direction as for a single crystal sample. In the case when vectors of normal to the slip plane, the slip directions, and the tensile axis are not coplanar, then traces of rotation are not pass through [101], but moving on arc of a circle defined by the equation obtained for proposed model. This case of rotation of the crystal lattice of a polycrystal grain is fundamentally differs from the rotation of a single crystal sample.

3. Based on the results of studying the surface of deformed samples by optical and electron microscopy, it was shown that, in most cases, dislocation slip in grains of two-dimensional polycrystalline aluminum foils with a "pancake" grain structure under active tension at room temperature occurs mainly in one primary slip system, which, presumably due to the absence of constraint of the grain structure and plastic deformation along the thickness of the sample. Experimental data of the tensile axis rotation traces (based on the results of X-ray diffraction determination of the crystallographic orientation of grains before and after deformation) indicates good agreement with the calculated data for the rotation traces of the tensile axis due to the action of the primary slip system.

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