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Computer indexing Laue diffraction pattern, the determination of the crystallographic orientation of the grains relative to the main directions in the crystal and the Schmid factor for all slip systems

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We describe a technique of computer indexing Laue patterns, determining the crystallographic orientation of the single-crystal sample (or a single grain of a polycrystal) relative to the main directions in the crystal, and Schmid factors for all systems sliding without the use of construction of a stereographic projection of the normals to the reflecting planes.

The basic algorithm of this procedure is to define and build a system of unit vectors of the normals to the Laue diffraction pattern, and according to the terms of her shooting, similar to the definition of the radius vector to the crystallographic orientation of the crystal planes known, combining them into a single computer center and a reversal of these systems relative to each other before the match First the radius vector with a portion of the latter. Thus, the indices of the reflecting planes are determined to Laue spots. After the Laue diffraction pattern indexing program to determine the crystallographic orientation of the studied sample and Schmid factor values for all slip systems.

Keywords: computer technique, the unit vectors, crystallographic orientation, Schmid factor.

Описана комп›ютерна методика індиціювання лауеграмми, визначення кристалографічної орієнтації монокристалічного зразка (або окремого зерна полікристала) щодо основних напрямків у кристалі і факторів Шміда для всіх систем ковзання без використання побудови стереографічної проекції нормалей до відбиваючих площин.

Основним алгоритмом цієї методики є визначення та побудова системи одиничних векторів нормалей до відбиваючих площин за даними лауеграмми і умов її зйомки, аналогічні визначення системи радіус– векторів до кристалографічних площин відомої орієнтації кристала, суміщення їх в один центр і комп›ютерне розвертання цих систем відносно один одного до збігу перших радіус векторів з частиною останніх. Таким чином, визначаються індекси відбиваючих площин для лауеграмми. Після індіціювання лауеграмми програма дає можливість визначити кристалографічну орієнтацію дослідженого зразка та значення фактора Шміда для всіх систем ковзання.

Ключові слова: комп›ютерна методика, одиничні вектори, кристалографічна орієнтація, фактор Шміда.

Описана компьютерная методика индицирования лауэграмм, определения кристаллографической ориентации монокристаллического образца (или отдельного зерна поликристалла) относительно основных направлений в кристалле и факторов Шмида для всех систем скольжения без использования построения стереографической проекции нормалей к отражающим плоскостям.

Основным алгоритмом этой методики является определение и построение системы единичных векторов нормалей к отражающим плоскостям по данным лауэграммы и условиям ее съемки, аналогичные определения системы радиус – векторов к кристаллографическим плоскостям известной ориентации кристалла, совмещение их в один центр и компьютерный разворот этих систем относительно друг друга до совпадения первых радиус векторов с частью последних. Таким образом, определяются индексы отражающих плоскостей для лауэпятен. После индицирования лауэграммы программа позволяет определить кристаллографическую ориентацию исследованного образца и значения фактора Шмида для всех систем скольжения.

Ключевые слова: компьютерная методика, единичные вектора, кристаллографическая ориентация, фактор Шмида.

Introduction

It is well-known, that all crystaline bodies due to their structure are anisotropic, i.e. their physical properties depend on crystallographic direction. In most cases, it concerns mechanical properties. That is why, while researching pattern of development of plastic deformation and determining mechanical features of monocrystalline samples or separate grains of polycrystalls, the main condition is determining of their crystallographic orientation. For this reason, as a rule, a well-known X-ray Laue method is used[1]. The deciphering of lauegram, where each reflex (laue – spot) is a reflection of definite

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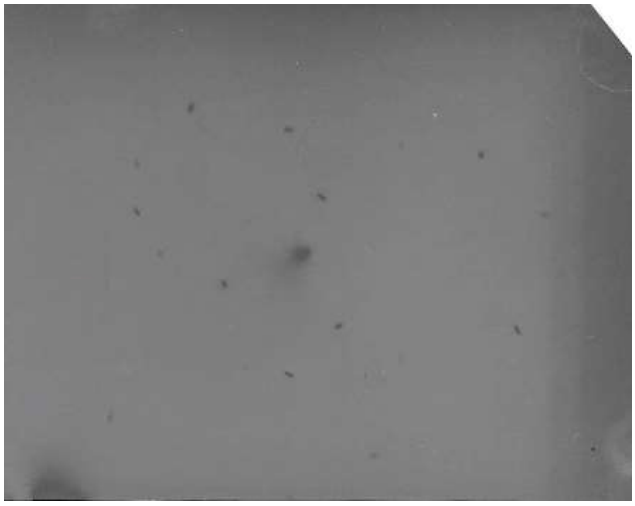
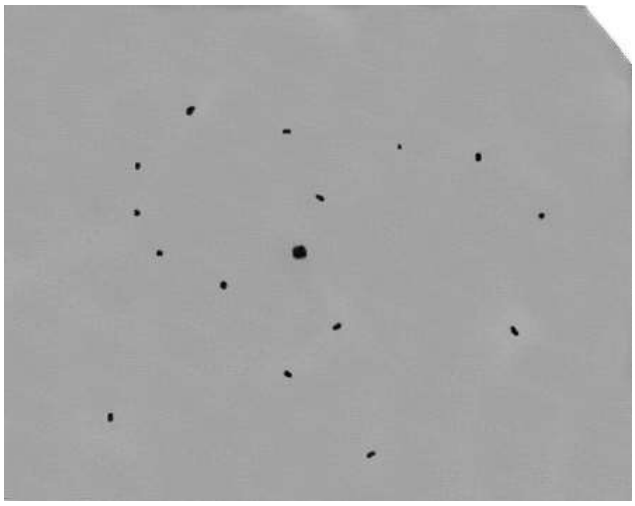
crystallographic plane with indexes (hkl), allows to determine crystallographic orientation of monocrystaline sample for separate grains of polycrystal in relation to the main directions in the crystal (for cubical crystals this is [001], [110], [111]).

Traditional and single method [2,3] of deciphering of lauegrams included building stereographic projection of normals to reflected planes with known indexes (according to the lauegram) and its comparison to similar stereographic projections of normal to planes with known indexes, built in advance, for crystals with different crystallographic orientation. This method is pretty demanding and not always gives unambiguous results.

Lately appeared the works [4], where the method that eliminates the building of stereographic projection of normals to reflections planes is described. The algorithm of this methodology is geometrical determination of angles between reflecting planes, taking into account the conditions, received with the help of lauegram, and their comparison with the angles between the directions of crystal bar with known indexes. This methodology greatly simplifies the procedure of indexing of lauegram, but it does not allow to completely automatize the method of determining crystallographic orientation of researched sample – monocrystalline.



a



b

Fig. 1. Images of scanned (a) and edited (b) lauegram, received from one of grains of polycrystalline.

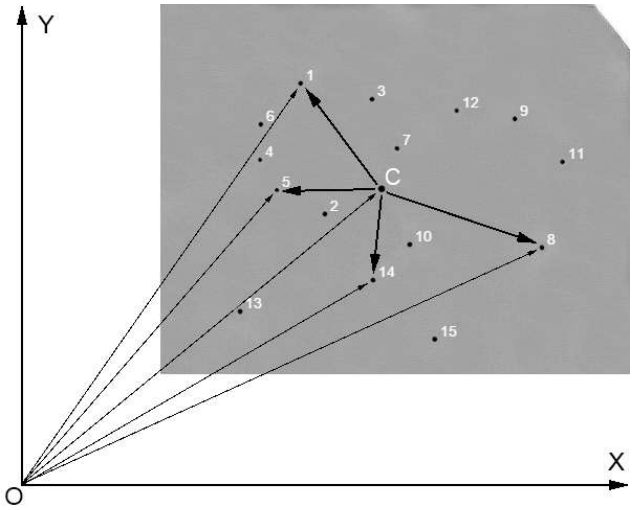


Fig. 2. The graph of building radius – vectors $\overrightarrow{on}$, $\overrightarrow{oc}$, $\overrightarrow{cn}$.

The aim of this article is to review and approbation algorithm of the method of indexing of lauegram and determining the crystallographic orientation of grain in relation to the main directions in the crystal and Shmidt`s factor for all glide systems.

Results and discussion

The algorithm of the method of indexing of lauegram and determining the crystallographic orientation of grain in relation to the main directions in the crystal and Shmidt`s factor for all glide systems.

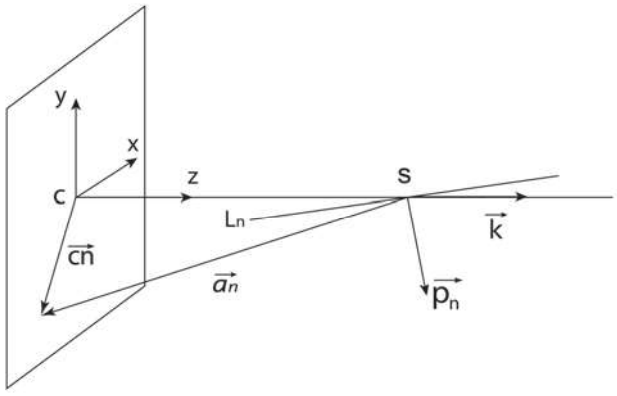


Fig. 3. The graph of building single vectors of normal $\vec{P}_n$ to reflecting planes: S- sample; Ln – reflecting plane, $\vec{k}$ – is unit vector of the axis Z.

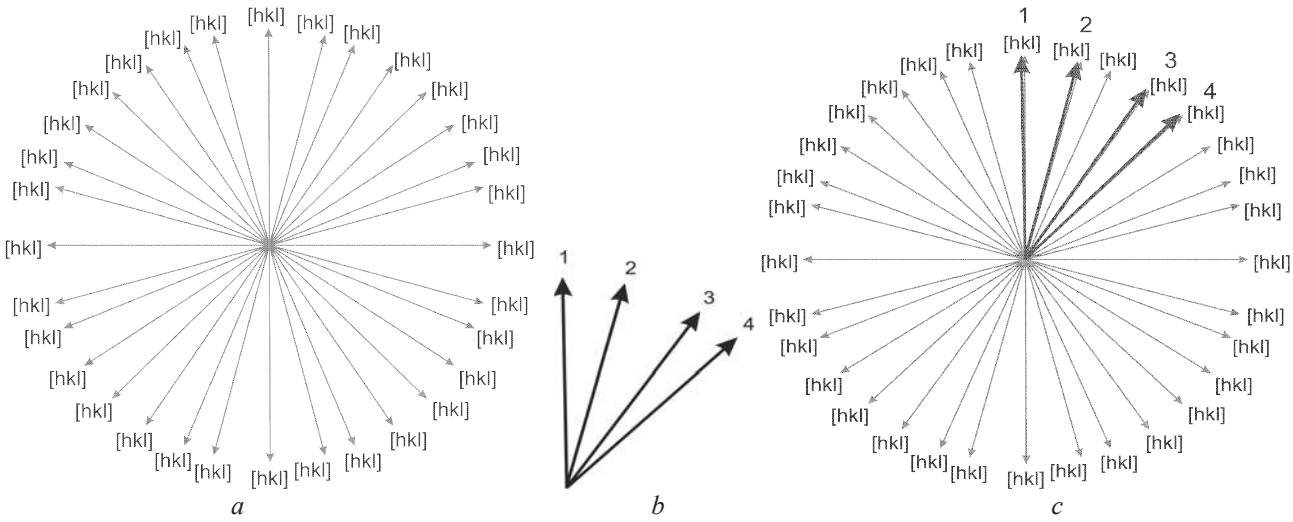


Fig. 4. Single radius – vector of normals to crystallographic planes with given indexes $\vec{P}_{hkl}$ (a), reflecting planes $\vec{P}_n$ (based on data from lauegram) (b) and results of their comparison (c).

Above is shown the description of computer method, which allows in automatic mode to index lauegram, determine crystallographic orientation of the sample relative to the main directions in the crystal and the number of Shmidt`s factor for all glide systems.

The preparatory stage of this method is scanning of obtained lauegram, its editing to determine weak reflexes and storing it in one file. In figure 1, as example, the lauegram before (a) and after (b) editing is shown.

Further, the orthogonal system of numbers is presented of axis XYZ, where X – is direction of axis of stretching (the bottom part of the film), Z – is the direction, opposite the X-Ray bunch and the numbering of the reflexes of lauegram (n) and its center (c) is made (Fig.2).

The next stage is determining the radius – the vector of laue spots $\overrightarrow{on}$ and $\overrightarrow{oc}$, the vectors $\overrightarrow{cn}$ ($\overrightarrow{cn} = \overrightarrow{on} - \overrightarrow{oc}$), and their coordinates (Fig. 2) and determining single vectors of normals to surrounding planes ($\vec{P}_n$) for laue spots. The diagram of this determining is shown in figure 3.

From the figure we can see that if the distance sample–film (H) is known, the unit vector of normal to reflecting plane Ln can be determined by the following method:

$$\vec{P}_n = \frac{1}{\left| \frac{\overrightarrow{a_n}}{\overline{a_n}} + \vec{k} \right|} \left(\frac{\overrightarrow{a_n}}{\overline{a_n}} + \vec{k} \right), \qquad (1)$$

where $\overrightarrow{a_n} = \overrightarrow{cn} - H \cdot \vec{k}$, $\vec{k}$ – is unit vector of the axis Z, n – is the number of laue spots.

Determination of similar unit radiuses-vectors for planes with known indexes (hkl) for researched crystal is made by the formula:

$$\vec{P}_{hkl} = \frac{1}{\sqrt{h^2 + k^2 + l^2}} \begin{bmatrix} h \\ k \\ l \end{bmatrix}, \qquad (2)$$

where h, k, l = 0, ±1,±2,…,±n.

The last stage of this method is graphic building of unit radiuses – vectors $\vec{P}_n$ and $\vec{P}_{hkl}$ (Fig. 4.a, b, c) with common center.

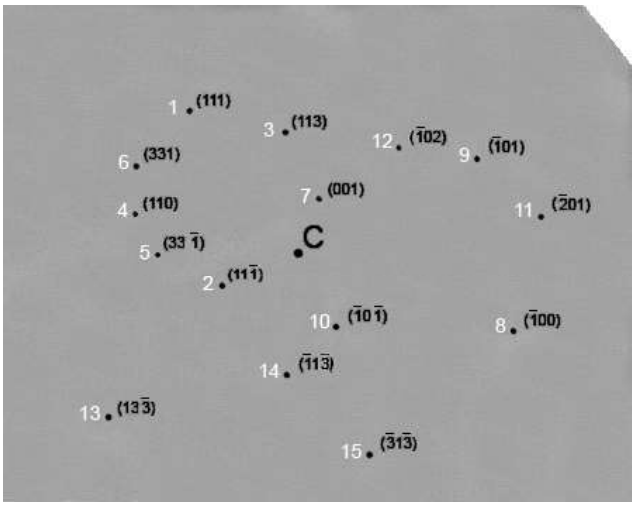


Fig. 5. Results of indexing of lauegram.

Computer program allows to find optimal common place of specters of vectors $\vec{P}_n$ and $\vec{P}_{hkl}$ in the space, which leads to co-inciding of vectors $\vec{P}_n$ with part of vectors $\vec{P}_{hkl}$, so that it allows each laue spot to allocate indexes to reflecting plane (hkl) (Fig. 5).

If on the lauegram there are no reflexes from crystallographic planes, normals, to which they are the

main crystallographic directions, they are determined based on the results of indexing of the lauegram, taking into account known angle correlation in crystalline bar between directions. Determining of vectors $\vec{P}_{100}$, $\vec{P}_{110}$, $\vec{P}_{111}$ in the system X,Y,Z, connected to the crystal allows to determine angle correlation between X,Y,Z and $\vec{P}_{100}$, $\vec{P}_{110}$, $\vec{P}_{111}$ (table 1).

Table 1

	[100]	[110]	[111]
X	32	24	20
Y	19	28	31
Z	24	35	23

Finally, using the correlation for determining Shmidt`s factor (m = cosα·cosφ, where α – is the angle between direction of axis of stretching and glide plane, φ – angle between normal to glide plane and direction of axis of stretching) (Fig. 6) can be determined Shmidt`s factor for all glide systems (table 2): $(\bar{1}11)[0\bar{1}1]$, $(\bar{1}11)[101]$, $(\bar{1}11)[\bar{1}\bar{1}0]$, $(\bar{1}\bar{1}1)[1\bar{1}0]$, $(\bar{1}\bar{1}1)[101]$, $(\bar{1}\bar{1}1)[011]$, $(111)[\bar{1}01]$, $(111)[0\bar{1}1]$, $(111)[1\bar{1}0]$, $(1\bar{1}1)[\bar{1}01]$, $(1\bar{1}1)[011]$, $(1\bar{1}1)[\bar{1}\bar{1}0]$.

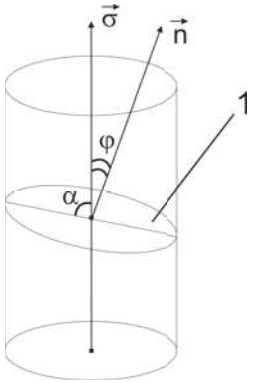


Fig. 6. The graph of determining Shmidt`s factor: 1 – glide plane (one of the planes {111}); $\vec{\sigma}$ – axis of stretching of sample; $\vec{n}$ – normal to the glide plane, φ – angle between the normal to the glide plane and direction of axis of stretching, α – angle between the direction of the axis of stretching and glide plane.

It should be mentioned, that offered method does not require difficult process of building and using stereographic planes.

Table 2

Glide systems	**1**	**2**	**3**	**4**	**5**	**6**
Shmidt`s factor	0,46	0,37	0,35	0,30	0,27	0,21
Glide systems	**7**	**8**	**9**	**10**	**11**	**12**
Shmidt`s factor	0,17	0,16	0,09	0,06	0,05	0,01

Conclusion

1. Computer method is developed, which allows to index lauegram, determine crystallographic orientation of monocrystallines (separate grains of polycrystalline) relative to the main directions in the crystal and Shmidt`s factor for all glide systems.

2. The main algorithm of this program is determining and building the system of single radiuses – vectors of normal to reflection planes (based on data of lauegram), system of similar vectors for crystals with known orientation and combination of their centers.

3. Computer program allows to determine the optimal common place of specters of these vectors in the space, which leads to maximal co-incidence of vectors, so that it allows to each laue spot to allocate indexes to reflection plane.

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