Relative misorientations of crystals

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Abstract. Orientation relationships between crystals are considered on the base on disorientation distribution function. The distribution of limit disorientation angles is obtained taking into account the symmetry of crystals. Maximum values of limiting disorientation angles for some crystallographic axis are calculated. Distribution density of disorientation angles corresponding to formation of coincidence site lattices is considered. Estimations of interphase disorientations between cubic and hexagonal crystals are carried out.

1. Introduction
Most of the currently used industrial materials are polycrystalline, whose properties are determined not only grains but also the grain boundaries [1]. Grain boundaries connecting by orientation relationship, leading to occurrence coincidence site lattice (CSL) have extreme properties associated with the grain boundaries energy, precipitates at the grain boundaries, grain boundary migration, slip along the grain boundaries, etc. [2]. The crystallographic texture describing the direct pole figures, inverse pole figures and orientation distribution function (ODF), characterizes the polycrystalline ensemble applied to the selected sample external coordinate system.
For a description of orientation relationship between the crystals is necessary to consider the misorientation distribution function (MDF).

2. Results and discussions
Since the relative orientation of the two grains may be given by matrix $g$ with a misorientation angle of rotation $\alpha$ and the axis of rotation $l$ or Euler angles $\varphi, \theta, \psi$, then misorientation can be seen or in the crystallographic space angle $\alpha$ - axis $l$, or in the Euler space. If we express the components of $g$ matrix through the angle $\alpha$ and the direction cosines of the axis of rotation $l$, then matrix $g$ takes the form of

$$
g(l, \alpha) = \begin{vmatrix}
l_1^2(1 - \cos \alpha) + \cos \alpha & l_1l_2(1 - \cos \alpha) - l_3 \sin \alpha & l_1l_3(1 - \cos \alpha) + l_2 \sin \alpha \\
l_1l_2(1 - \cos \alpha) + l_3 \sin \alpha & l_2^2(1 - \cos \alpha) + \cos \alpha & l_2l_3(1 - \cos \alpha) - l_1 \sin \alpha \\
l_1l_3(1 - \cos \alpha) - l_2 \sin \alpha & l_2l_3(1 - \cos \alpha) + l_1 \sin \alpha & l_3^2(1 - \cos \alpha) + \cos \alpha
\end{vmatrix}.
$$

When considering a grains misorientation as a function $g (l, \alpha)$ performs a misorientation matrix $A_0$, so that the equivalent misorientation matrices $A_i$ due to the symmetry of the crystal are found as

$$A_i = A_0 R_i^{-1},$$

where $R_i^{-1}$ - the elements, inverse to elements $R_i$ group pure rotation of the crystal.
Each element of the group has one and only one inverse element, so if $R_i$ takes all values elements of the group pure rotation, the $R_i^{-1}$ also takes all the values of the elements of the same group, but in a different order. Given this

$$A_j = A_0 R_j,$$

where $R_j$ - one of the elements of the corresponding group pure rotation.

Thus, for description of a misorientation of the two grains in a cubic material with the symmetry group O there exists 24 equivalent descriptions. The maximum possible value of the minimum rotation angle around the axis $u$ with crystallographic indexes $[mnp]$ is called the limit rotation angle $\alpha_{\text{lim}}$ around $[mnp]$. If the rotation angle $\alpha > \alpha_{\text{lim}}$, perhaps equivalent the description of the misorientation angle $\alpha_{\text{lim}} < \alpha$.

Figure 1 shows the distribution of the misorientation limit angles for cubic crystals (symmetry group O). In cubic crystals, limiting rotation angle for the $<100>$ is $45^\circ$, for $<110>$ - $\approx 61^\circ$, for $<111>$ - $60^\circ$. The maximum value of limit rotation angle for cubic crystals is equal to $\approx 62^\circ$ around $<221>$.

![Figure 1. Limit misorientation angles for cubic crystals.](image1)

![Figure 2. Limit misorientation angles for hexagonal crystals.](image2)

![Figure 3. The density distribution of the misorientation angles $P(\alpha)$ for cubic crystals.](image3)

![Figure 4. The density distribution of the misorientation angles $P(\alpha)$ for hexagonal crystals.](image4)

In the hexagonal crystals for the axis [0001] $\alpha_{\text{lim}} = 30^\circ$, for axes $<2\overline{1}0>$ and $<1\overline{1}0>$ $\alpha_{\text{lim}} = 90^\circ$, axes $<3\overline{2}0>$ $\alpha_{\text{pr}} = 92^\circ$. The maximum value of limit rotation angle for the hexagonal crystals $93^\circ50$ for axes $<1\overline{4}3\overline{5}>$ (figure 2). For a polycrystalline aggregate of all misorientation angles is a sphere of radius $\pi$. Turn in this case is determined by the vector length $l$ along the axis $\alpha$, predetermined angles $\theta$ and $\varphi$. To determine the density distribution of the misorientation angles $P(\alpha)$ must perform invariant
integration [3] by parameters \( \theta \) and \( \varphi \), setting the position of the axes of a reversal, within the scope of the area of the minimum misorientation:

\[
P(\alpha) = \frac{(1 - \cos \alpha) \int_{\theta} \sin \theta d\theta d\varphi}{4\pi^2}.
\]  

(4)

This integration corresponds to the area of the section calculation field \( V_E \) of minimum misorientation angle by sphere of radius \( \alpha \).

Figure 3 and figure 4 show the density relative misorientation angles distribution \( P(\alpha) \) for the cubic and hexagonal crystals.

Under certain strictly fixed values of the axis and rotation angle neighboring crystals (ratio Kronberg-Wilson) occurs coincidence site lattice (CSL). To characterize the CSL often use the reciprocal coincidence site lattice density, denoting by \( \Sigma \) - number of lattice points per one coinciding node and the number \( \Sigma \) always simple. So \( \Sigma = 1 \) means a complete coincidence lattices and no border. At \( \Sigma = 3 \) occurs a double in the FCC lattice. Special properties of grain boundaries are preserved under small deviations of the lattices neighboring grains relative orientation from the special. The maximum deflection angle (in radians) of a special orientation, which could possibly lead accommodation using dislocations and grain boundary are saved special properties defined as

\[
\Delta \alpha = \frac{10 \div 15}{\pi \sqrt{\Sigma}}.
\]  

(5)

If for description of crystal misorientations using parameters such as the angle \( \alpha \) and the axis of a misorientation \( \mathbf{u} \), then set of all possible misorientations can be represented as a sphere of radius \( \pi \). The volume of the misorientation space as the orientation space with Euler angles is \( 8\pi^2 \).

Figure 5 within the standard stereographic triangle shows the distribution of misorientations corresponding to emergence of coincidence site lattices to \( \Sigma = 99 \) for cubic crystals.

![Figure 5](image)

**Figure 5.** Distribution of misorientations corresponding to emergence of coincidence site lattices to \( \Sigma = 99 \), for cubic crystals.

Figures 6 and 7 show the misorientation distribution corresponding to emergence of coincidence site lattices on the sides of the standard stereographic triangle for cubic and hexagonal crystals.
In the case of interphase misorientations the misorientation matrix $A_k$ has the form $A_k = R_i A_0 R_j$, where $R_i$ and $R_j$ are the elements of crystal symmetry the respective phases and $A_0$ is the misorientation matrix of the respective phases.

Distribution of the limit angles interphase misorientations for cubic and hexagonal crystals is shown in figure 8. The density of the interfacial misorientation angles $P(\alpha)$ of cubic and hexagonal crystals is shown in figure 9.
3. Conclusions
The limit misorientation angles and the misorientation angle distributions for the cubic crystals and the hexagonal crystals were determined. The angles corresponding to appearance of the coincidence site lattices for $\Sigma = 99$ cubic crystals and $\Sigma = 25$ hexagonal crystals were determined within the standard stereographic triangle. The limit angles of interfacial misorientation and the distribution of misorientation angles for cubic and hexagonal crystals were calculated.

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References
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