Double bragg reflections in single crystals and textured polycrystals

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Abstract. Analysis of the detection of the double Bragg reflections (DBR) in single crystals and polycrystals is carried out. Technique of the detection of the double Bragg reflection in single crystals and textured polycrystalline samples using X-ray synchrotron radiation is proposed.

1. Introduction
Sufficient full description of polycrystalline material suggests the knowledge not only the texture but relative crystal misorientation, since many physical and mechanical properties as high-temperature creep, grain boundary diffusion, grain boundary corrosion, grain boundary sliding depends of relative orientation of crystallites [1, 4]. Traditional X-ray texture analysis allows determining the orientation of the crystal relative to the selected external system of coordinates associated with the sample. The possibility of determining the relative orientation of the crystals in a polycrystalline sample is opened by using the double Bragg reflections [2, 3].

2. Double Bragg reflections
The effect of double Bragg reflections originally discovered in single crystals. Thus, the Renninger effect is to observe in diamond forbidden diffractive reflection 222 by sequential reflections from planes (311) and (1).

In general, the Laue interference equation for reflection from the plane \( (h_1k_1l_1) \) is given by

\[
\frac{s_1-s_0}{\lambda} = H_1,
\]
and for reflection from a plane \( (h_2k_2l_2) \):

\[
\frac{s_2-s_0}{\lambda} = H_2.
\]

After subtracting the second from the first relation we have

\[
\frac{s_1-s_2}{\lambda} = H_{12},
\]
where

\[
H_{12} = H_1 - H_2.
\]

Equation (3) shows that \( s_0 \) ray, reflected from the plane \( H_2 \), again reflected from the plane \( H_{12} \), goes in the direction \( s_1 \). Thus, in the case of single crystals of FCC and BCC metals the double Bragg reflections are superimposed on the basic reflection that does not permit them to watch. Using the X-ray synchrotron radiation polarized in the horizontal plane allows to extinguish the reflection \( (h_1k_1l_1) \) in the horizontal plane by choosing a wavelength \( \lambda \) with \( 2\theta = 90^\circ \) to reflect \( (h_1k_1l_1) \). Now,
implementation of equations (1) and (2) allows to register the double Bragg reflection $H_{12}$, which corresponds to the "internal" of double Bragg reflections in single crystals. In the polycrystalline samples possible "external" double Bragg reflections, which carry information about the intergranular misorientations. In this case, relation (1) holds for the first crystal, and the ratio of (2) - for the second. Now $H_1$ is reciprocal lattice vector of the first crystal, and $H_2$ - of the second and $H_{12}$ is:

$$H_{12} = H_1 - R_{12}H_2,$$  

(5)

where $R_{12}$ - orientation matrix for the second crystal relative to the first.

3. Results and discussions

Knowing the orientation distribution function (ODF) or the analysis of direct pole figures of the polycrystalline sample allows you to select two peaks with orientation matrices $R_1$ and $R_2$, which corresponds to the matrix of crystals misorientation $U_{12} = R_2^{-1}R_1$. Figure 1 a, b shows the geometry of the "external" double Bragg reflection, at first from the plane $n_1(h_1 k_1 l_1)$ at an angle of Bragg $\theta_1$ for crystal 1, and then the plane $n_2(h_2 k_2 l_2)$ at an angle of Bragg $\theta_2$ for crystal 2. On the stereographic projection, the center coinciding with the normal to the sample surface $N$ (figure 1 c), showing the outputs of normals $n_1(h_1k_1l_1)$ and $n_2(h_2k_2l_2)$, which are the axes of the diffraction cone with half-angles $\pi / 2 - \theta_1$ and $\pi / 2 - \theta_2$ for the first and second crystals respectively.

The intersection of the circles corresponding to these cones, determines the general direction of $s_1$, which allows to find the direction of the primary beam $s_0$ and the direction of double reflected beam $s_{12}$. Now, the angle $\varphi$ between $N$ and $s_0$ determines the installation angle of the sample $\pi / 2 - \varphi$ between the primary beam $s_0$ and a normal to the sample surface, and the angle $\psi$ between $N$ and $s_0$ -

![Figure 1](image-url)
installation angle for the detector on a diffractometer. Position of the plane passing through \( s_0 \) and \( s_{12} \), determines the installation tilt angle \( \eta \) of the sample for recording double Bragg reflections in the equatorial plane at the texture attachment for diffractometer. The intensity of the detected reflection proportional to the probability distribution function of the main peak misorientations for a polycrystalline sample.

4. Summary
The use of synchrotron X-ray radiation provides the following advantage: weak DBR can be easier revealed due to the improved signal/background ratio. Optimum wave length of a primary monochromatized radiation can be selected taking into account an average grain dimension (for polycrystals) and X-ray radiation attenuation coefficients \( (\mu_\lambda) \). Double Bragg reflections can find application in investigation of mutual misorientations of interphase boundaries, including the case of considering orientation relationships at phase transformations.

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