Combined texture and microstructure analysis of deformed crystals by high-energy x-ray diffraction

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Supplementary Material

Transformation of the ROI intensity from detector frame to the pole figure

Equation (3) in the main paper describes the transformation of the diffraction vector from the laboratory frame to the sample frame. For calculating the pole-figure angles (the polar angle ψ with regard to ND and the azimuthal angle φ, with regard to RD) corresponding to detector coordinates $(2\theta, \eta)$ and the rotation angle ω it is better to rewrite eq. (3) in terms of unit vectors along $\boldsymbol{G}_S$ and $\boldsymbol{G}_\omega$:

$$\boldsymbol{e}_S = \mathbf{S^{-1}}\boldsymbol{\Omega}_z^{-1}\boldsymbol{e}_\omega. \tag{SM-1}$$

where $\boldsymbol{e}_S = \frac{\boldsymbol{G}_S}{|\boldsymbol{G}_S|}$ and $\boldsymbol{e}_\omega = \frac{\boldsymbol{G}_\omega}{|\boldsymbol{G}_\omega|}$. Considering $\boldsymbol{S} = \boldsymbol{I}$, eq. (SM-1) changes to:

$$\begin{pmatrix} \sin\psi\cos\varphi \\ \sin\psi\sin\varphi \\ \cos\psi \end{pmatrix} = \cos\theta\,\boldsymbol{\Omega}_z^{-1}\begin{pmatrix} -\tan\theta \\ -\sin\eta \\ \cos\eta \end{pmatrix}. \tag{SM-2}$$

Since $\boldsymbol{\Omega}_z^{-1}$ rotates around Oz does not change the 3rd component of the vector on the left hand side, which leads to the following relation for the polar angle ψ:

$$\cos\psi = \cos\theta\cos\eta. \tag{SM-3}$$

The equations relating the first two components of the vectors in eq. (SM-2) give the azimuthal angle of the pole figure:

$$\tan\varphi = \frac{\sin\omega\sin\theta - \cos\omega\sin\eta\cos\theta}{-\cos\omega\sin\theta - \sin\omega\sin\eta\cos\theta} \tag{SM-4}$$

Table S1. The parameters of the diffraction geometry obtained according to the procedure of Borbély *et al.*(2014).

parameters	Distance [mm]	Beam centre [pixel]		Detector normal components		
		u	*v*	n_1	n_2	n_3
initial	730.0	735.0	830.0	1	0	0
calibrated	734.47(2)	736.50(3)	831.77(5)	0.999972(3)	0.00692(6)	0.00248(6)

Table S2. The set of ω angles corresponding to the Bragg condition of 111 type diffraction vectors, belonging to two variants of the S3 texture component: $(1,2,3)[6,3,-4]$ and $(1,-3,2)[6,4,3]$ (the corresponding Euler angles $\varphi_1, \phi, \varphi_2$ are: 301.020°, 36.699°, 26.565° and 152.968°, 57.689°, 161.565°, respectively). The Table shows that the set of ω angles does not depend on the (*h'k'l'*)[*uvw*] choice of the texture component. All 24 equivalent definitions lead to the same set (only two are presented).

Diffraction vector	ω [°]	
h,k,l	$(1,2,3)[6,3,-4]$	$(1,-3,2)[6,4,3]$
1 1 1	274.65	76.74
1 1 1	109.49	251.15
-1 1 1	322.43	7.4
-1 1 1	135.32	181.52
1 -1 1	1.52	274.65
1 -1 1	187.4	109.49
1 1 -1	76.74	315.32
1 1 -1	251.15	142.43
-1 -1 1	71.15	322.43
-1 -1 1	256.74	135.32
-1 1 -1	7.4	289.49
-1 1 -1	181.52	94.65
1 -1 -1	315.32	1.52
1 -1 -1	142.43	187.4
-1 -1 -1	289.49	71.15
-1 -1 -1	94.65	256.74

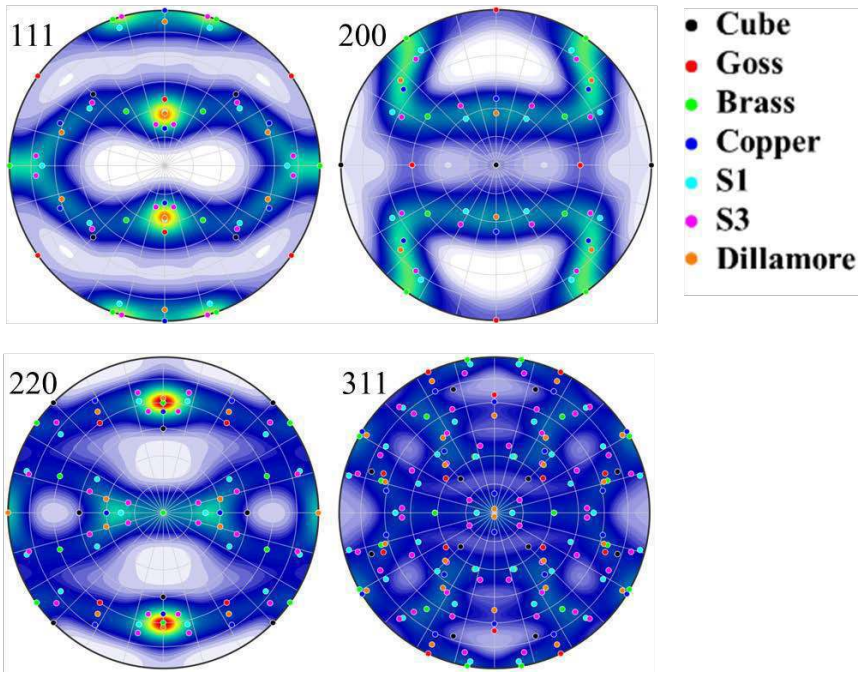
Table S2 shows the relation between the selected grain orientation (*h'k'l'*)[*uvw*] and the corresponding dislocation contrast factors for two variants of the S3 component: $S' = (1,2,3)[6,3,-4]$ and $S'' = (1,-3,2)[6,4,3]$. The average contrast factor is usually calculated based on *a priori* information on the relative populations of the crystal slip systems, which can be estimated from crystal plasticity calculations (Borbély *et al.*, 2000) or from experimental TEM analysis. To exemplify the link between the selected grain orientation (***U***) and the dislocation contrast factor we show an example based on Schmid factors. This approximation may be valid for uniaxial tension and small strains, when one expects that the majority of dislocations belong to the slip system with the highest Schmid factor. Applying the force along the longitudinal direction [6,3-4] and [6,4,3] respectively, the largest Schmid factor of 0.422, corresponds to the slip systems (1-1-1)[110] and (11-1)[101] for the S' and S'' variants, respectively. Considering 50% edge and 50% screw type dislocations the mean $\bar{C}_{hkl}$, can be calculated by averaging the individual contrast factors, which can be numerically calculated according to the anisotropic theory of elasticity. The results were obtained with the *AnizC* software (Borbély et al., 2003) using the following second order elastic constants $\mathbf{C}_{11}$ = 107 GPa, $\mathbf{C}_{12}$ = 60.8 GPa and $\mathbf{C}_{44}$ = 28.3

GPa. The *AnizC* is freely available at http://metal.elte.hu/anizc/. It is important to note that the spots always appear at the same $(2\theta, \eta, \omega)$ coordinates, however, their notation (200, 020 or 002) should be done according to the variant used for the Schmid factor calculation.

Table S3. The (η, ω) coordinates and average contrast factors of 200 type diffraction vectors corresponding to beam energy of 63 keV.

(η, ω) [deg]	S'	$\bar{C}_{hkl}$	S''	$\bar{C}_{hkl}$
(30.0, 302.3)	0 0 2	0.0119	2 0 0	0.2835
(129.8, 285.5)	0 2 0	0.2835	0 2 0	0.0119
(63.2, 216.6)	-2 0 0	0.2835	0 0 2	0.2835

Figure S1 Location of the 111/222, 200, 220 and 311 diffraction vectors of the selected texture components in the sample frame (PF). The selected poles are mostly lying in regions with high density, excepting the Cube and the Goss components.



References

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