X-RAY DIFFRACTION

Analysis of highly textured metal sheets using elliptical components in DIFFRAC.TEXTURE

Application Note 625

Texture modeling brings orientation analysis from qualitative glances at pole figures to quantitative values required for process control of modern materials. The traditional mathematically derived harmonic approach is useful for the generation of complete pole figures and transformation of coordinate system into ODF and inverse pole figure space, but leaves analytical values locked within a list of obscure coefficients. The component approach allows direct modeling of the morphology based on fundamental materials and process variables, thereby giving researchers a direct connection between the modeled result, crystallographic orientation, and process direction.

In the component method texture is modeled using a combination of elliptical, spherical, and fiber components. Spherical components exhibit a uniform spread in the orientation distribution in a specific direction while a fiber models a component which is highly oriented in one direction and random in the orthogonal direction. Elliptical components are the most general case with the ability to adjust the spread in the orientation distribution along three axes.

This application note discusses the use of elliptical components to describe the texture in a sheet of molybdenum metal.

Experimental Details

Data were collected on a D8 DISCOVER diffractometer (see Figure 1) equipped with a Cu tube operating at 40 kV, 40 mA, a parallel beam polycapillary lense, a 500 µm UBC collimator, a centric Eulerian Cradle, and an EIGER2 R 500K detector operating in 2D mode in the gamma-optimized orientation. To increase detector angular coverage the sample to detector distance was set to 150 mm. A similar configuration is also available in the D8 ADVANCE.

To obtain pole figures, 2D frames were taken as continuous scans in ϕ (the azimuthal angle) at successive values of ψ (the tilt angle).

The large coverage in γ and 2θ reduces the number of required ψ steps significantly enhancing measurement speed compared to a 0D or 1D method. In this experiment (110) was collected in 2 ψ steps (see Figure 2) while (200) and (211) were collected in 3 ψ steps. A thinned algorithm was used with a nominal angular resolution of 5° in ϕ.
At 5 s per frame, the total data collection time was 30 min for all three pole figures. Frame data were imported into DIFFRAC.TEXTURE where pole figures were quickly generated and fit using the component method, assuming monoclinic process symmetry.

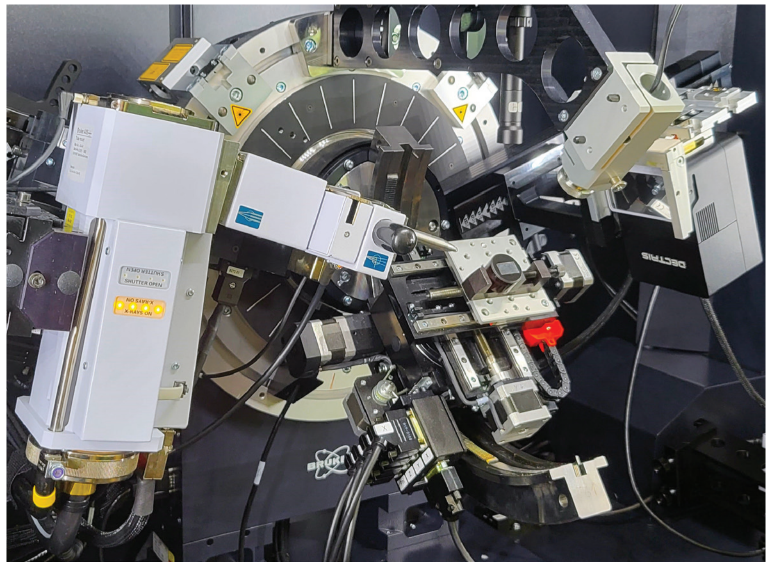


Fig. 1 D8 DISCOVER configured for the measurement of pole figures.

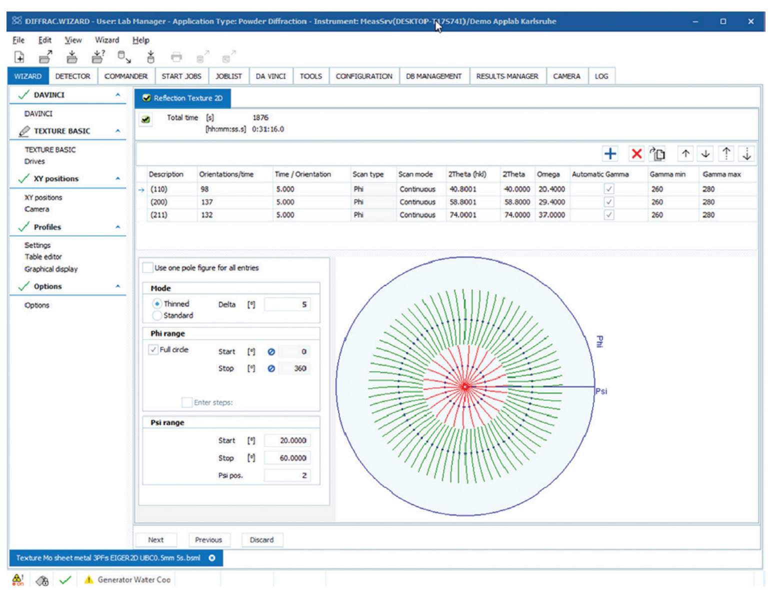


Fig. 2 Pole figure measurement planning in DIFFRAC.WIZARD.

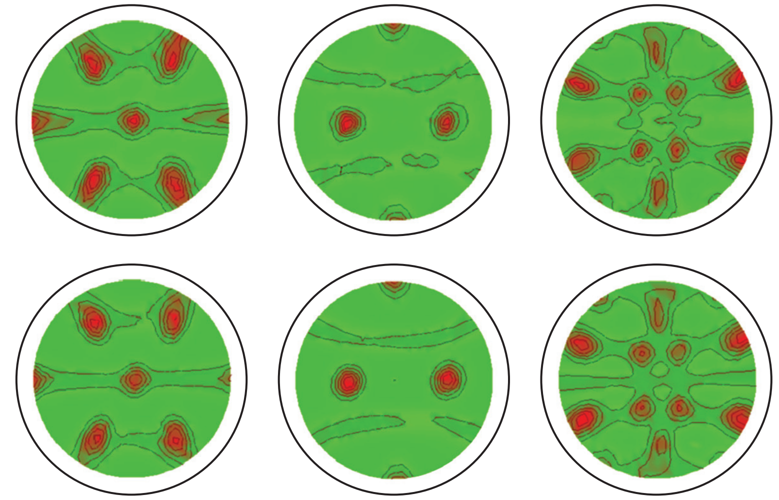
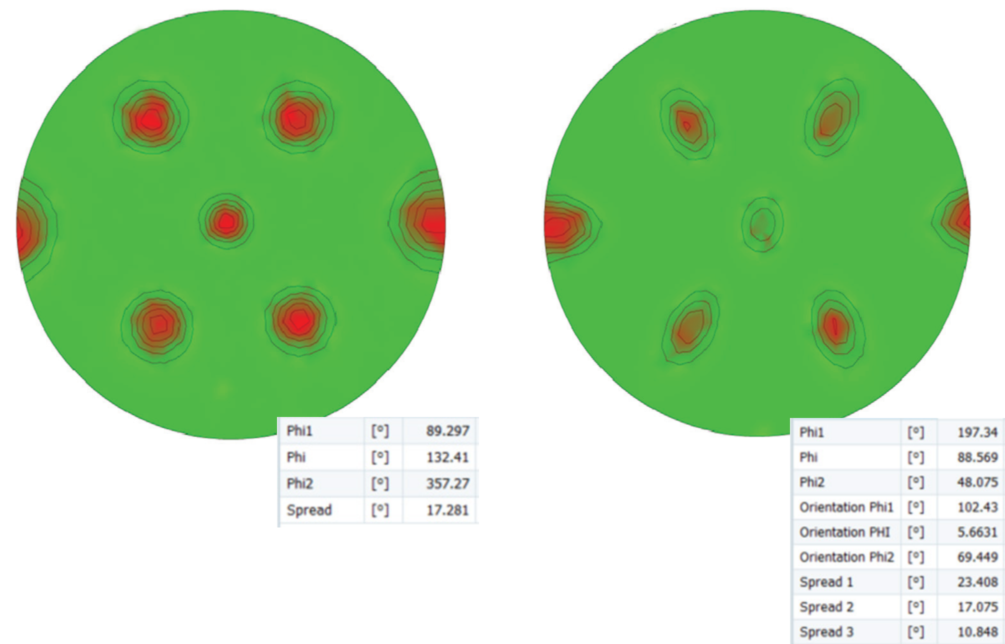


Fig. 3 Experimental (top) and recalculated (bottom) (110), (200) and (211) pole figures of the molybdenum sheet metal.

Results

Figure 3 shows the experimental and recalculated pole figures for the Mo sheet metal. The analysis was performed by fitting the pole figures using the component method based on two components. The first component is nearly spherical but only the elliptical component can address the slightly elliptical shape of the orientation distribution. This can be visualized by looking at the recalculated (110) pole figure of the first used elliptical component (Figure 4, right).

The anisotropic distribution of the pole density is clearly visible. The possibility to refine spreads in three independent directions allow a precise refinement of the experimental pole figure. For comparison the recalculated (110) pole figure based on a spherical component is shown in (Figure 4, left). Here we see the isotropic spread of the spherical component that provides only a limited representation of the experimental situation.



Phi1	[°]	89.297
Phi	[°]	132.41
Phi2	[°]	357.27
Spread	[°]	17.281

Phi1	[°]	197.34
Phi	[°]	88.569
Phi2	[°]	48.075
Orientation Phi1	[°]	102.43
Orientation PHI	[°]	5.6631
Orientation Phi2	[°]	69.449
Spread 1	[°]	23.408
Spread 2	[°]	17.075
Spread 3	[°]	10.848

Fig. 4 Recalculated (110) pole figure using a single spherical (left) and elliptical (right) compo-nent. The table shows the additional degrees of freedom allowed for elliptical components.

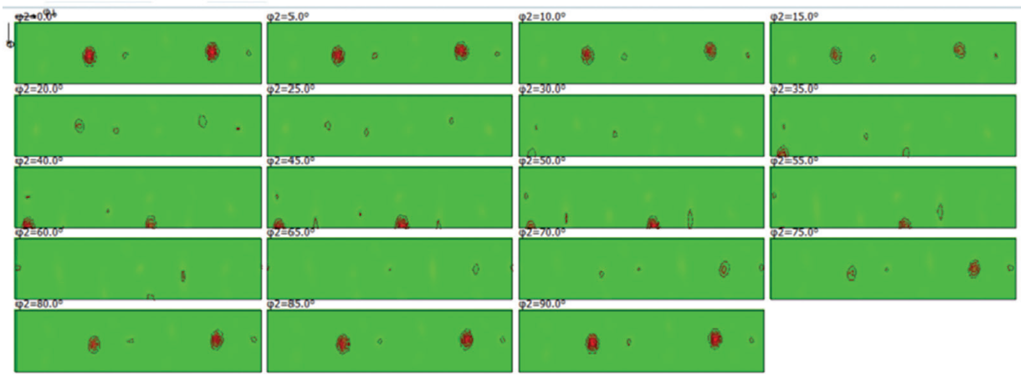


Fig. 5 Orientation distribution function (ODF) for the molybdenum sheet metal.

The orientation distribution function (ODF) is a statistical description of the preferred orientations of grains in a material. Figure 5 shows the ODF plotted in constant sections of the Euler angle ϕ2. The inverse pole figure (Figure 6) is often used by process engineers to directly correlate crystallographic orientation and process conditions with the rolling (RD), transverse (TD) and normal directions (ND) of the physical sample. For this sample, a strong (101) orientation exists in the rolling direction and strong (001) and (111) orientation in the transverse direction. The normal direction, the thin direction of the sheet metal, shows a strong (101) orientation with a weak lean into the (113) orientation.

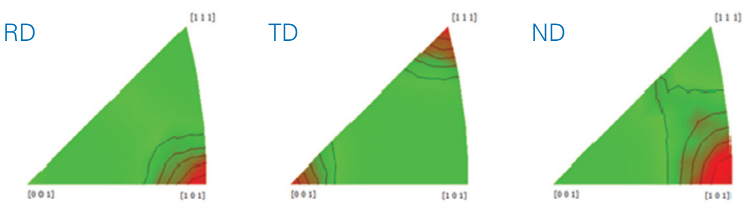


Fig. 6 Inverse pole figure (IPF) obtained for the molybdenum sheet metal.

Summary and Conclusion

In this application note the texture of a Mo sheet metal was analyzed using a D8 diffractometer and DIFFRAC.TEXTURE.

- The combination of the EIGER2 detector and the intelligent planning in DIFFRAC.WIZARD allows the collection of three high quality pole figures in 30 minutes.
- The pole figures reveal the anisotrophic texture of the sheet metal. Elliptical components in DIFFRAC.TEXTURE are perfectly suited to model such textures and a single component is sufficient to fully describe the measurements.

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