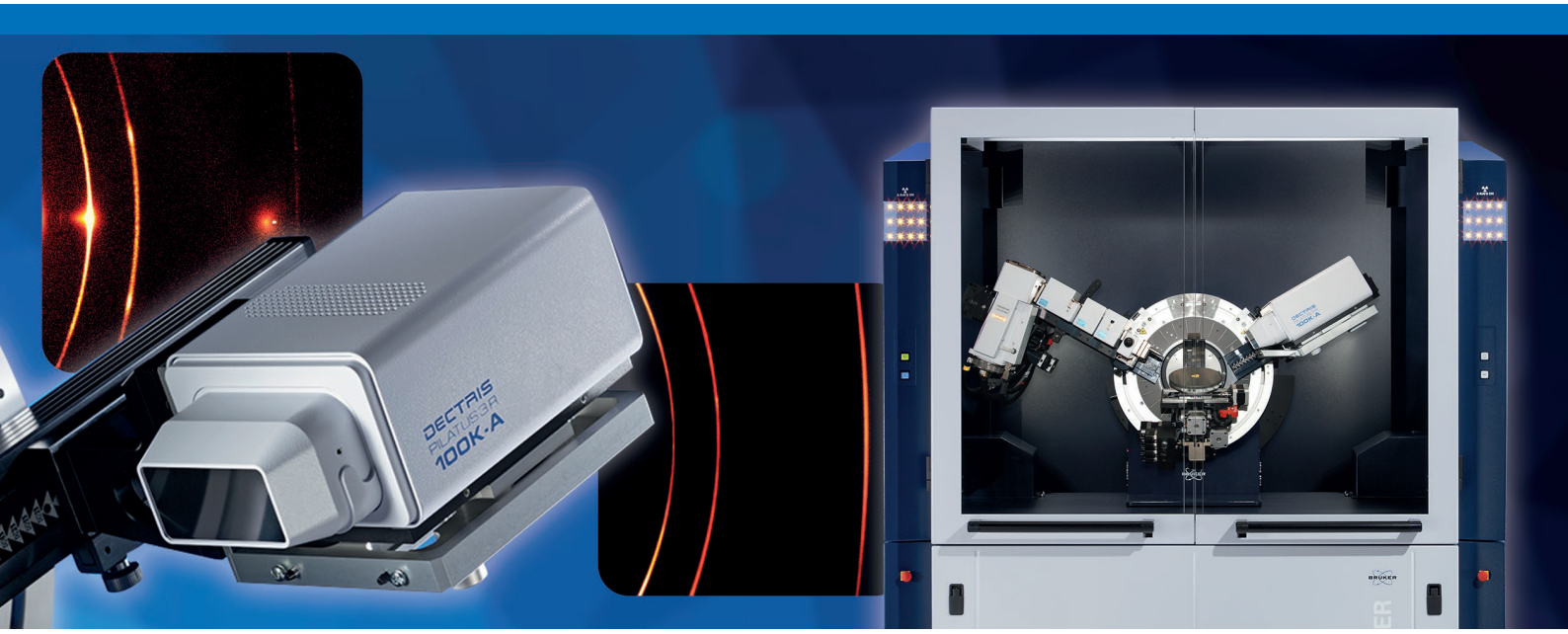

Application Report XRD 23

D8 DISCOVER with PILATUS3 R 100K-A Texture Analysis with XRD²

The D8 family of diffraction solutions combined with the DECTRIS PILATUS3 R 100K-A detector is an innovative 2D x-ray diffraction (XRD²) solution that is uniquely suited for multi-purpose modern materials research characterization. In this report, we present the capabilities of this system combined with DIFFRAC.TEXTURE analysis software for investigating the texture in metal samples.

Introduction

The macroscopic properties of a material are closely linked to the way in which its microscopic crystallographic grains are arranged. By creating a strong preferred orientation, properties can be enhanced, but at the same time, the material can become more susceptible to catastrophic fracture. The orientation of the grains is commonly referred to as its texture. With XRD this is probed by measuring the intensity as a function of tilt and rotation of several crystallographic reflections, creating a map called a pole figure. The measured pole figures can be modeled with respect to the crystallographic symmetry of their associated reflections to determine the texture of a sample, known as the orientation distribution function (ODF). For some analyses, the ODF is the end result, but in other cases, reconstructed pole figures or inverse pole figures based on the ODF are required.

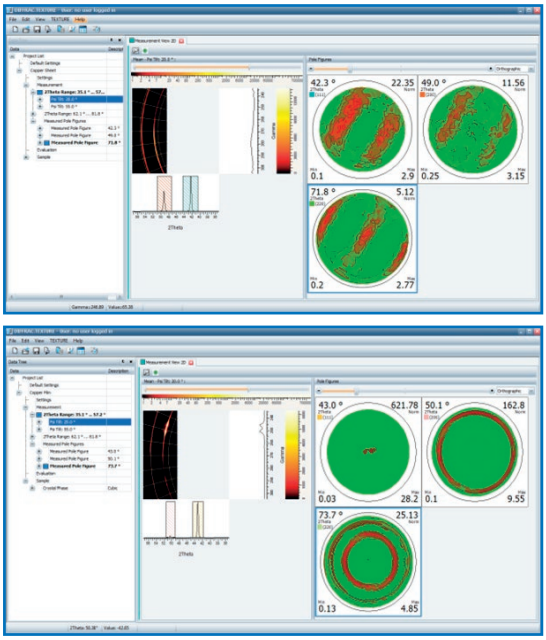

Figure 1: Pole Figure Creation in DIFFRAC.TEXTURE of a Copper Sheet (top) and a Copper Film on Si (bottom.)

Measurement

A thin copper sheet and a 1 µm copper thin film on silicon substrate were investigated. The samples were measured in reflection with a D8 DISCOVER equipped with a copper IµS micro-focus source, 300 micron collimator, a centric Eulerian cradle and PILATUS3 detector positioned 10 cm from the sample. The detector was mounted in a gamma optimized orientation to increase the tilt coverage of the measurement.

For texture analysis, pole figures from a minimum of 3 non-collinear reflections are required. For this analysis, the (111), (200) and (220) reflections of copper were used. In order to cover the pole sphere, 2 sets of frames were collected. The first set covers both the (111) and (200) reflections with $2\theta = 45^\circ$, $\Psi = 20^\circ$, 55°, and $\phi = 0$ to 360° in 5° increments resulting in 144 frames. The second set covers the (220) reflection with $2\theta = 72^\circ$, $\Psi = 15^\circ$, 40°, 65°, and $\phi = 0$ to 360° in 5° increments, resulting in 216 frames. Each image was collected for 10 seconds, resulting in a total collection time of 1 hour.

Results

The frames were loaded into DIFFRAC.TEXTURE, where the (111), (200) and (220) pole figures were generated, as shown in Figure 1. The pole figures were then modeled using the spherical harmonic method.

The copper sheet shows a fairly complex texture, likely resulting from a rolling process used to produce the material. Although the ODF, shown in the middle of Figure 2, seems quite complex, it represents a classic rolling texture. The inverse pole figure of the copper sheet, shown in the bottom image of Figure 2, shows a strong (011) orientation normal to the surface and a weak (112) component in the normal direction.

In contrast, the copper film shows a fairly simple texture, consisting of 2 fibers. This is shown as 2 spots near the center of each slice of the ODF, the middle image of Figure 3. From the inverse pole figure, it can clearly be seen that the majority of the grains are (111) oriented in the direction normal to the film surface, while there is very weak orientation in the in-plane rolling and transverse directions. The PILATUS3 detector for XRD[2] combined with DIFFRAC.TEXTURE software makes texture analysis fast and simple.

Author

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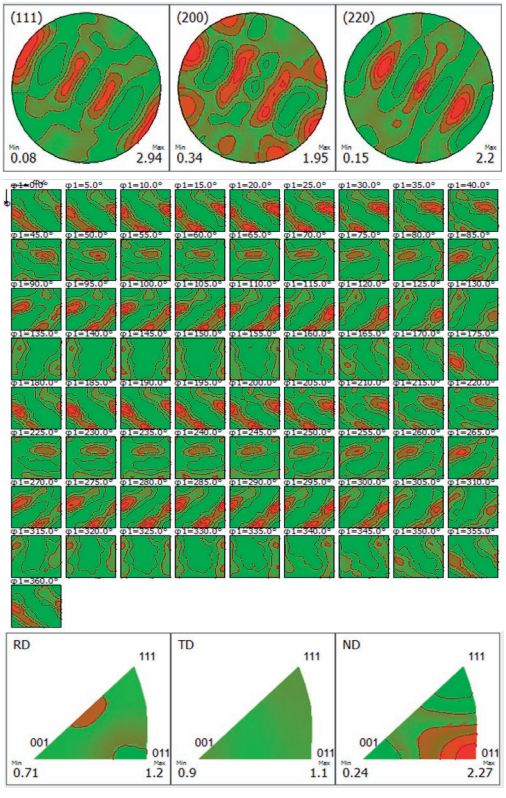

Figure 2: Results of DIFFRAC.TEXTURE Analysis of a Copper Sheet; Reconstructed Pole Figures (top), ODF (middle), Inverse Pole Figure (bottom).

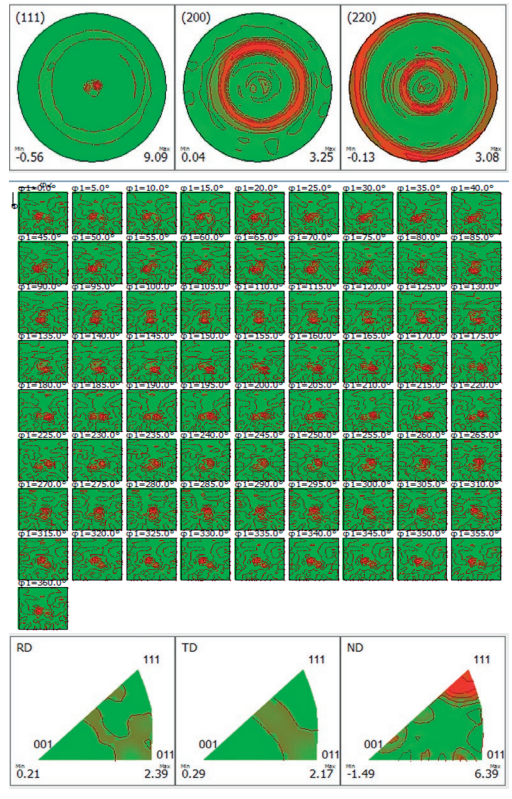

Figure 3: Results of DIFFRAC.TEXTURE Analysis of a Copper Film on Si; Reconstructed Pole Figure (top), ODF (middle), Inverse Pole Figure (bottom).

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