Parallel Beam X-Ray Diffraction

X-ray diffraction provides the only non-destructive measuring technique to determine residual stresses in materials.

Polycapillary optics are well suited for powder diffraction. The primary advantage of the collimating optic is a parallel beam in two directions, which significantly reduces systematic errors in peak position and intensity. In addition, both orientation and counting statistics can be improved by ten to one-hundred times relative to parallel-beams formed by parallel apertures.

**POLYCAPILLARY COLLIMATING OPTICS FOR STRESS AND TEXTURE ANALYSIS**

**FIGURE 1**

These pole figures show a comparison of Bragg-Brentano geometry and a parallel beam produced by a 2D polycapillary collimator. The 2D collimator greatly enhances the diffracted intensity for very thin layers (typically 3-100 Å thick) and weak reflections. The signal-to-noise ratio is increased by 10 to 20 times, thus allowing rapid data collection. Furthermore, accurate measurements from tilted specimen are improved because the beam is collimated in both the horizontal and vertical directions.

**FEATURES:**
- Small or large beam size
- Large capture angle of x-rays
- 2-D collimated parallel beam
- Large intensity gain
- Constant peak profile over entire 2θ range
- Easy alignment of optic

**BENEFITS:**
- Analysis of irregularly shaped, “realworld samples,” like crankshafts, turbine blades, wafers, etc.
- No defocusing errors even at high sample tilts
- In-line applications can eliminate inefficient off-line sample preparation
- Integration with small-spot sources
- Insensitive to sample displacement and transparency

100Å Ag on Si 111 Pole Figure

Data measured at BEDE Scientific Inc., Denver, CO
POLYCAPILLARY COLLIMATING OPTICS FOR STRESS AND TEXTURE ANALYSIS

The polycapillary optic collimates the beam in two dimensions eliminating asymmetric peak broadening. These optics provide a nearly perfect Gaussian peak shape with constant instrumental broadening over the entire 2θ range.

The superior quality of the parallel-beam geometry is clearly seen, especially at high ψ angles. No peak shifting occurs over the whole ψ-range; even at high ψ angles useful intensity can be collected. This allows very high-precision residual stress and texture analysis, with the ability to accurately map reciprocal space.

An intensity gain of 40X is obtained with the polycapillary optic compared to a measurement with Bragg-Brentano Geometry.

Data measured at BEDE Scientific Inc., Denver, CO
Phase ID and Quantitative Analysis

Enhance instrument performance with collimating polycapillary optics for Parallel-Beam Powder Diffraction from X-Ray Optical Systems, Inc. These lenses are ideally suited for industrial applications, full pattern analysis, and integration with microfocus sources.

**FIGURE 4**
Comparison of effects on peak positions as a function of sample displacement for Parallel-Beam and Bragg-Brentano geometry

*In Parallel-Beam Geometry no peak shifts occur.*

**Table of Benefits:**
- No peak shifts due to sample displacement or specimen transparency
- Eliminates Bragg-Brentano Geometrical Constraints
- Measure irregularly shaped, rough samples
- Minimizes or eliminates sample preparation
- Measurements unaffected by sample tilts
- Improved counting statistics
- Improved orientation statistics

Data measured at KRATOS Analytical, Chestnut Ridge, NY
PHASE ID AND QUANTITATIVE ANALYSIS

**FIGURE 5**
Determination of the surface coating of an Advil® tablet

An x-ray diffraction scan of an “off the shelf Advil® tablet” reveals a sugar coating on the surface after matching the pattern with ICDD card 24-1977 (Sucrose). This demonstrates the excellent capability of the polycapillary optic to measure irregular samples.

**FIGURE 6**
Quantitative Phase Analysis of NIST SRM 8486 Portland Cement Clinker

Constant peak shape and width were achieved with the polycapillary optic making the data ideally suited to full-pattern analysis. The diagram shows the comparison between the raw data and the full-pattern fit for quantitating phase analysis. The measured data in Table 1 shows good agreement with NIST data.

**TABLE 1**
Analysis data of NIST SRM 8486

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<thead>
<tr>
<th>Phase</th>
<th>NIST Data</th>
<th>Measured</th>
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<tr>
<td>Alite</td>
<td>58.47%</td>
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<tr>
<td>Belite</td>
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<td>21%</td>
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<tr>
<td>Aluminate</td>
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<td>Ferrite</td>
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<td>Periclase</td>
<td>3.21%</td>
<td>4%</td>
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<tr>
<td>Total %</td>
<td>99.69%</td>
<td>100%</td>
</tr>
</tbody>
</table>

The World Leader in X-Ray Optics

XOS® offers standard and custom designs for your analytical needs.