TEAM™ WDS Element Scan Simplifies Peak Separation and Trace Element Detection Analyses

Element Scan
WDS optimization using the Element Scan routines allows the user to tailor data collection specifically to a particular goal: fine peak separation or trace element detection. The microanalysis data required to solve each of these goals differs and, in the past, an advanced level of knowledge was required to set up the WDS in order to capture the relevant data. Now, using the TEAM™ WDS software, these parameters are set automatically once the user identifies the element and energy line of interest and clicks on the analysis goal.

<table>
<thead>
<tr>
<th>If your goal is</th>
<th>What you need is</th>
<th>TEAM™ software provides</th>
</tr>
</thead>
<tbody>
<tr>
<td>PEAK SEPARATION</td>
<td>Best resolution</td>
<td>Element Scan with Better Resolution setting</td>
</tr>
<tr>
<td>TRACE ELEMENT DETECTION</td>
<td>Highest intensity</td>
<td>Element Scan with Higher Intensity setting</td>
</tr>
</tbody>
</table>

EDS / WDS Comparison
A sample analysis is required of a fluorinated surface layer on an iron part. Unfortunately, the energy of Fe L lines are very close to the energy of the F K X-rays which produces an overlap situation. Figure 1. The use of a high resolution X-ray spectrometer like WDS is needed to resolve the F K and the Fe L lines.

The diffractors in WDS collect X-rays over a range of energies. Depending upon the diffractors mounted in the WDS spectrometer, small energy ranges exist at the edges of these ranges where two or more potential diffractors can be used to collect X-rays. The selection process for the “best” diffractor can seem complicated, but is usually delineated into Peak Separation and Trace Element Detection acquisitions.

Peak Separation and Trace Element Detection
For a Peak Separation task, the diffractor that provides the best spectral resolution is preferred; whereas, for a Trace Element Detection task a diffractor with the highest sensitivity (intensity) is preferred. If multiple diffractors are an option, the one with the larger d-spacing is preferred for trace analysis while the one with the smaller d-spacing is preferred for peak separation.

As seen at the bottom of the Element Selection screen shown in Figure 2, the analyst has selected to analyze the sample for Fe and has a choice of two diffractors (D3 and D4) for the L line, and one (D1) for the K line. If the goal of the analysis is peak separation and the L line is chosen, the TEAM™ WDS software will automatically choose the D4 diffractor, which will give results with the best resolution. If the goal is trace element detection, the D3 diffractor will be used, giving the highest intensity.

The WDS Elemental scans for each of these diffractors is shown in Figure 3 using the same vertical scaling. The intensity of the D3 diffractor is significantly higher than that of the D4 diffractor. This observation is not so important for the high F K peak but is significant in identifying the much lower intensity Fe L lines. However, the spectral resolution using this diffractor does not fully separate the F K, Fe Lα1 and Fe Lβ1 peaks. Use of the D4 diffractor more clearly separates each of these peaks, especially the Fe Lα1 and Fe Lβ1 peaks, for visual identification but at a reduced intensity.

Conclusion
As advances in microanalytical hardware technology improve performance, precise software optimization becomes increasingly more important. The Element Scan routines within the TEAM™ WDS software guarantee the best data collection possible, allowing all users to achieve the highest level of insight into their material.