

AN INNOVATIVE EDXRD PROBE

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Energy Dispersive X-Ray Diffraction (EDXRD) provides a number of distinct advantages for the detection and verification of materials. Unlike Angular X-ray Diffraction (AXRD), which uses a monochromatic beam, EDXRD uses a “white” x-ray beam to probe the samples. No moving parts are necessary; source, sample, and detector positions are fixed. With an energetic beam the x-rays can penetrate through relatively thick materials and diffract from crystalline sample materials within a defined diffraction region. The sample materials can be identified even when they are located within opaque, sealed containers. That is, for many cases, samples without any sample preparation can be located and examined even when hidden in other materials.

XStream Systems, Inc has developed a table top EDXRD system that fits a number of applications. The table top unit uses a confocal geometry to maximize the x-ray intensity from a relatively low-powered, air-cooled 80 kV x-ray source. The beam is collimated by a circular slit assembly before the sample. A similar slit assembly after the sample collimates the diffracted beam and defines the diffraction region. A single CdTe solid-state detector with a multichannel analyzer is used to process the diffracted signal. This collimation system allows us to interrogate a doughnut-shaped volume within the sample under test. In addition, the confocal geometry provides an effective gain of more than 200 times over that of a simple, single beam system with the same resolution.

One of the design goals for the instrument was to develop a unit that is capable of performing quick verification or detection of complex materials such as pharmaceuticals and, yet can be operated by personnel with minimal scientific knowledge. The rapid identification of unknowns is possible using advanced pattern matching techniques, such as neural networks and other pattern matching algorithms. A localized SQL database is used to store a Material Recognition Software Engine’s (MRSE) library of material detectors. The MRSE is capable of matching an unknown sample’s spectrum to a known material’s spectrum by first processing the raw data and then performing pattern matching. This engine has demonstrated that it can verify a number of drugs, each in less than 5 min, to better than a 97 percent accuracy.

The current application of the system has been directed toward the verification of pharmaceuticals in sealed containers. The theory of operation and examples of data of various drugs will be discussed in the paper. Techniques to apply the unit to analysis and other applications will also be shown.