# **RAPID II**

DIMAX RAPIDI

The most versatile 2D micro-diffraction system in the world

D/MAX RAPID II is arguably the most versatile micro-diffraction XRD system in the history of materials analysis. In production for well over a decade and continuously improved during that time period, the success of the D/MAX RAPID II is a testament to the suitability of imaging plate technology for measuring diffraction patterns and diffuse scattering from a wide range of materials.

### **Engineered for Versatility**

It combines an exceptionally large active-area imaging plate that is sensitive to a wide range of radiation sources with the flexibility to mate it with a large variety of X-ray sources and optics. The nature of the imaging plate detector means that weak measurements can be made easily in the presence of strong measurements.

#### Low Cost of Ownership

Combining a well-proven, time-tested design with the lack of a need for calibration means that the RAPID II is a detector that can be maintained in the field with a minimum of downtime.

### The Proof is in the Results

Experiments run on the RAPID II are limited only by the imagination of the researcher. Examples include, phase ID of powder samples, micro-diffraction mapping down to 10 microns, diffuse scattering, fiber diffraction, small molecule structure analysis, stress and texture measurements, etc.

### Features

- Curved imaging plate provides a large 210° aperture
- Long exposures allowed because of absence of dark current noise
- Large dynamic range achieved with dual photomultiplier design.
- High sensitivity coupled with low readout noise.
- Imaging plate detector sensitive for all potential X-ray targets
- Multiple X-ray source options, from sealed tube to rotating anode generators
- No detector calibration required.
- Low maintenance—all components can be serviced on-site.
- Huge experimental versatility, from powders to single crystals.

#### **Application:**

#### Non-uniform crystalline state of a PET bottle

Plastic bottles must have strength to resist heat and mechanical shock, and these strengths are said to depend on the degree of crystallinity and stretching orientation. A two-dimensional X-ray diffraction image directly reveals information about preferred orientation and the crystalline state of a sample. If the orientation of the molecules is random, the diffraction image is ring-shaped; however if some preferred orientation is present, the image is in the shape of an arc.

### Crystallization of a rubber band by stretching

When a piece of rubber is pulled it extends and when it is released it shrinks back to its original length. The macroscopic ability of rubber to stretch under a small force (elasticity) originates from a change in the microscopic molecular structure. An orientational difference in the alignment of the molecules arises between the pulling direction and the direction perpendicular to that in which the rubber is being stretched. A two-dimensional diffraction image collected on an R-AXIS RAPID II shows these effects simultaneously.

### Solution structures and precrystallisation molecular association

Nucleation—the initial stage of crystal growth—is a challenging area to study experimentally, but an understanding of the process is essential as increasing numbers of important materials are found to exhibit polymorphism, even when grown under seemingly identical conditions. To examine the assembly of potential supramolecular building blocks in crystallization processes, this study focuses on initial molecular assembly in the solution state; knowledge of this early stage assembly can help understand the dominance of certain polymorphs in the crystalline state.

### Comparing cellulose in Sitka spruce and in celery

Wood is a material of immense technological importance, and is ubiquitous in everyday life. As well as a fuel, it has been an important construction material since humans

began building shelters, houses and boats, and it is enjoying renewed importance in construction as an environmentally sound and sustainable material. The uses of a particular type of wood are entirely dependent on its physical properties, but despite its economic importance, the structure of wood that underlies these physical properties is still poorly understood.

#### Software:



PDXL is a one-stop full-function powder diffraction analysis software suite. The modular design, advanced engine and user-friendly GUI have been satisfying both experienced and novice users since PDXL was released in 2007.

PDXL provides various analysis tools such as automatic phase identification, quantitative analysis, crystallite-size analysis, lattice constants refinement, Rietveld analysis, ab initio structure determination, etc.

### Fundamental parameter method

The peak shape in a powder diffraction pattern would appear to be a delta function if measured under ideal conditions. In reality, the peak shape changes depending on a number of measurement conditions: wavelength distribution of the source, optical systems, slit conditions, crystallite size and strain, and so on. The peak shapes obtained from measurements made under real-world conditions are described using an empirical function such as a split pseudo-Voigt function, or a split Pearson VII function which has a good agreement with the obtained peak shapes. The fundamental parameter method (FP method) is a method to calculate peak shape by convolution of the shapes caused by all the instrumental and sample conditions.

# Phase identification using COD

The Crystallography Open Database (COD) is a free, public-domain database of the crystal structures published in International Union of Crystallography, Mineralogical Society of America and so on. PDXL can incorporate both ICDD/PDF-2 and COD to perform automatic phase identification, adding the COD library of over 150,000 crystal structures to PDXL 2's already substantial capabilities.

# Wizard for ab initio crystal structure analysis

Recently, there have been many published examples of ab initio crystal structure analysis performed on powder diffraction data. This development is attributed primarily to significant improvements in PC processing speed and in the efficiency of the algorithms used for structure determination.

PDXL has so far provided all of the functions required for ab initio crystal structure analysis, such as indexing, structure determination and structure refinement by the Rietveld method. Now the "Structure Analysis Wizard" is available in PDXL to provide support and guidance for users undertaking the complicated procedure of structure analysis, particularly of organic compounds. This wizard system will make it possible for even the beginner to achieve analytical success

### **Clustering function**

The PDXL clustering feature can group multiple scan data based on the similarity of powder diffraction patterns and peak positions, and displays the grouped data in an easy-to-read tree. This is particularly effective when it comes to classifying and screening the data from a large number of scans.