FA5-MS40-P01

Combined X-ray Micro-Diffraction, Radiography and Tomography Analysis of Solid Objects. Detlef Beckers[a], Gabriel Blaj[a], Herbert Pöllmann[b], Klaus Bethke[a], Roger Meier[a], [a]*PANalytical, Almelo, The Netherlands,* [b]*Martin –Luther University of Halle, Mineralogy, Germany*
E-mail: detlef.beckers@panalytical.com

In this contribution, we will show examples of the strength of the combination of X-ray (micro-) diffraction, X-ray imaging and Computed Tomography (CT) results on solid objects. New developments – especially in detector technology – allow integration of these techniques on one laboratory X-ray diffraction system. By combining phase analysis with density and microstructure information a complete picture of the sample is obtained. Results can be correlated with macroscopic material properties. Examples from building materials, natural objects and pharmaceutical tablets are shown.

Keywords: Computed tomography, imaging, X-ray diffraction

FA5-MS40-P02

Development of a high brilliance rotating anode dual-wavelength X-ray generator and multi-layer mirror for dual-wavelength. Akihiko Iwata [a,c], Claire Wilson [a], Akihito Yamano [b], Masataka Maeyama[b], [a]*Rigaku European Headquarters, Berlin Germany* [b]*Rigaku Corporation, Tokyo Japan,* [c]*Kyoto University, Kyoto Japan*
E-mail: iwata@rigaku.co.jp

Due to growing demand for the use of different characteristic X-ray wavelengths such as Cu K-alpha and Mo K-alpha for crystal structure determination, dual X-ray source (DS) diffractometers have been widely used lately. However, DS diffractometers use sealed X-ray tube technology, and the X-ray intensity is limited with sealed tube X-ray generators. Still demands for using high intensity and different wavelengths X-ray for structure determination for very tiny crystals and low diffraction efficiency crystals exist. Since the middle of the twenty century, many challenges in developing a rotating anode dual wavelength generator have been overcome to achieve high intensity different characteristic X-ray wavelengths from a single X-ray generator. [1]
We have developed a new rotating anode X-ray generator which is capable of generating two different characteristic X-ray wavelengths without target exchanges. The electron beam can excite the two different target materials plated on a single rotating anode, as the anode can move in the X-ray tube housing under vacuum atmosphere. The newly developed optics unit consists of two confocal multi-layer mirrors, one for Cu K-alpha and the other one for Mo K-alpha, mounted in a single optic component face to face. The optics unit has a unique mechanism to switch between the two different characteristic X-ray wavelengths, details of which will be presented.

[1] Taylor, A.: Journal of Scientific Instruments. 26 (1949) 225.

Keywords: single crystal structure determination, dual-wavelength, high brilliance X-ray generator

FA5-MS40-P03

How tiny is a small crystal today? Holger Ott[a], [a]*Bruker AXS GmbH, Karlsruhe, Germany*
E-mail: info@bruker-axs.de

Instrumentation for single crystal structure analysis has advanced greatly over the last decade. These improvements include the introduction of area detectors, in particular CCD detectors with high dynamic ranges; as well as major software improvements.
For a number of years now systems using a flat graphite monochromator combined with a sealed tube source have been routinely used in laboratories in the western hemisphere. Although rotating anode generators using this monochromator were sparsely installed, they do allow for the measurement of smaller and more weakly diffracting crystals.
The introduction of multilayer mirrors opened the door for rationally designed X-ray optics. Originally these optics were available for wavelengths in the range of 1.54 Å or longer. More accurate control of the deposition process enabled mirrors for shorter wavelengths, down to 0.5 Å. These optics are widely used in microfocus X-ray sources and rotating anode generators using a variety of wavelengths and allow for measurement of tiny crystals. When allied with a high quality goniometer, exhibiting a small sphere of confusion, and a high-end CCD detector the minimum crystal size needed is pushed even further.
The presentation will focus on the recent progress in source development and suggest most suitable source-wavelength combinations based on carefully selected examples.

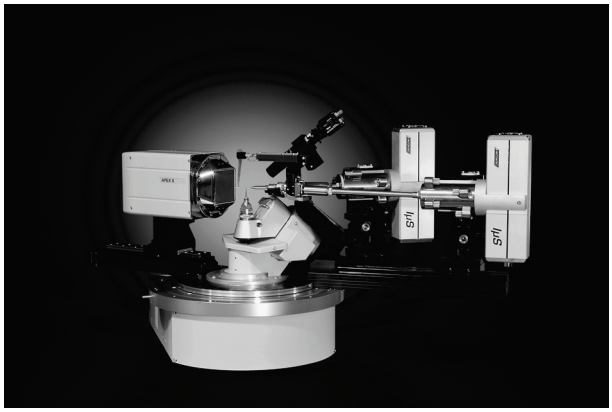

Figure 1: APEX DUO equipped with two micro focus sources

Keywords: Crystal size, Microfocus source, Single-crystal structure

FA5-MS40-P04

On the peak shapes of X-ray micro diffraction. Hejing Wang[a], Jian Zhou[b], [a]*School of Earth and Space Sciences, Peking University, P. R. China,* [b]*Chinese Academy of Geological Sciences, P. R. China*
E-mail: hjwang@pku.edu.cn

Since 1969 Rietveld [1] used the Gaussian function to model X-ray diffraction (XRD) peaks it has been a very common