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Acta Cryst. (2011) A67, C681**X-ray diffractometer with ellipsoidal multilayer mirror for convergent optics**

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Rigaku SmartLab is a multipurpose, fully-automated horizontal X-ray diffractometer that allows many types of applications. SmartLab's expandable system and the Cross Beam Optics (CBO) enable the realization of various optical configurations. The optics of the CBO system permits easy switching of incident X-rays by simply changing the selection slit. The Cross Beam Optics mechanism allows user selectable switching between two incident X-ray beam without resetting or realigning the optical system. Both system geometries are permanently mounted and permanently aligned to allow easy changeover for different applications.

In the Rigaku SmartLab two Cross Beam Optics systems are available: CBO and CBO-E. The CBO lets the user select the Bragg-Brentano focusing method or parallel beam method using the parabolic multilayer mirror, while the CBO-E lets the user select Bragg-Brentano focusing method or convergent beam optics using an ellipsoidal multilayer mirror. The convergent beam optics enables high resolution measurements by the transmission method. This method is used to measure samples with low absorption coefficients and preferred orientation, such as pharmaceuticals.

The Cross Beam Optics systems (CBO and CBO-E) can be combined with a Johansson type Ge crystal for monochromatization of the incident X-rays to the $K\alpha_1$ ($K\alpha_1$ system) [1]. One of the main applications of $K\alpha_1$ X-rays is powder pattern indexing of unknown crystal structures. Since the diffracted X-rays are not obstructed in the $K\alpha_2$, the separation of the overlapping Bragg reflections becomes easier in the $K\alpha_1$ system. The $K\alpha_1$ system is designed as the position of the focal point of the Johansson type crystal is corresponding to the conventional X-ray source. Due to the design of the $K\alpha_1$ system it acts like a virtual X-ray source. Therefore, the CBO or CBO-E system can be used in the same way as the conventional $K\alpha$ system. Consequently, the $K\alpha$ system and the $K\alpha_1$ system can be easily switched.

The diffracted X-rays can be focused on the detector plane by means of using $K\alpha_1$ monochromatized X-rays together with convergent-beam optics (CBO-E). If we consider this optical system, high-speed and high-intensity measurement can be realized, if the high-speed one-dimensional position sensitive X-ray detector D/teX Ultra is used.

In this presentation, we report outline of the optics on the Rigaku SmartLab system and discuss high-resolution measurement results by using CBO-E with and without $CuK\alpha_1$ system.

[1] *The Rigaku Journal (English version)*, 2010, 26(2), 29-30.

Keywords: X-Ray diffractometer, convergent-beam optics, powder diffraction

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Acta Cryst. (2011) A67, C681**Investigation structural of the new solid solution series: $Sr_{10-x}Nd_x(PO_4)_{6-x}(SiO_4)_xF_2$ ($0 \leq x \leq 3$) with rietveld method**

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Apatitic phosphosilicates, generally called "britholites" [1] have

been the object of a great interest because of their potential use for the conditioning of nuclear wastes [2]. They crystallize mainly in the hexagonal system (space group $P6_3/m$).

In this work, we present study structural of the new solid solution series of $Sr_{10-x}Nd_x(PO_4)_{6-x}(SiO_4)_xF_2$ ($0 \leq x \leq 3$). The structure has been determined at room temperature from X-ray diffraction by the Rietveld method analysis. A variation of the a and c lattice parameters in the solid solutions was observed, with a decrease of a and c parameters, related to the radius of the corresponding substituted ions. The structural refinement using the Rietveld method [3(a, b)] indicated that Nd^{3+} ions were located into the two sites with a strong preference for M(2) sites especially for low contents. A progressive shift of the F⁻ position along the c -axis outside the centre of the triangle formed by M(2) atoms was observed with the increase of x . Fourier maps were performed. These maps of electron densities expressed the existing possibility of each atom composing britholites. In particular, columnar neodymium and screw-axis neodymium were clearly revealed.

[1] J. Felsche, *J. Solid State Chem.* **1972**, 5, 266. [2] E. Du Fou de Kerdaniel and al., *J. Nucl. Mater.* **2007**, 362, 451-458. [3] a- H.M. Rietveld, *Acta Cryst.* **1967**, 22, 151. b- H.M. Rietveld, *J. Appl. Crystallogr.* **1969**, 2, 65.

Keywords: britholites, rietveld method, sites

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Acta Cryst. (2011) A67, C681-C682**Biodegradable polymer-clay nanocomposites**

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The use of conventional plastics in the last years has been broadened to new areas. Due to their low degradation rates, they can cause ecological problems when disposed as solid waste. Biodegradable polymers (BP) offer an alternative to keep sustainable development economically and ecologically attractive. Polyhydroxybutyrate (PHB) is an example of a BP, obtained from renewable resources. It has been found that polymers with nanostructured natural minerals enclosures lead to nanocomposites (NC) with highly improved stiffness, thermal stability, decreased flammability and gas-barrier properties at low loading (<5vol%). Addition of 5% of a functionalized commercial clay (30B-cloisite, 30BC, Southern Clay), by melt intercalation has yield a PHB NC with improved tensile modulus and better fire properties [1]. In spite of its many possible applications, its high melting point, brittleness, and low toughness, make their use difficult. Polycaprolactone (PCL), a synthetic BP, has a low melting point and is ductile at room temperature. The physical mixture of these polyesters is an alternative to obtain new materials with desirable properties. Blends of PCL and PHB are immiscible. Here we present the characteristics of NC produced by addition of 30BC to mixtures of PHB with PCL in different ratio. Samples were prepared in an intermeshing twin screw extruder. Films were obtained in a single screw extruder with flat die and take off unit. NCs were investigated by X ray diffraction (XRD) and differential scanning calorimetry (DSC). The results indicate that some degree of polymers insertion between the clay layers has been achieved. According to the literature [2] simultaneous small angle X-ray scattering (SAXS) and XRD studies yielded quantitative characterization of nanostructure and crystallite structure in some NC. Data from synthesized materials present the (001) diffraction peaks of the phyllosilicate almost at the same position as in the neat clay, along