s7.m0.p9 New Control Software for the KM6 Six-Circle Kappa Goniometer. M. Meyer[*†], A. Kowalski[‡], D. Kucharczyk[‡], W.A. Paciorek[•], G. Chapuis[*], [*]*Université de Lausanne, Institut de cristallographie, BSP, CH-1015 Lausanne;* [†]*Kuma Diffraction Instruments GmbH, PSE-B-1.5;* [‡]*Kuma Diffraction Ltd. Al. Akacjowa 15b, PL-53-122 Wroclaw;* [•] *Global Phasing Ltd., Sheraton House, Castle Park, Cambridge CB3 0AX UK.*
Keywords: diffractometer, instrumentation, CCD, 6-circle.

In 1996 Kuma Diffraction has created a 6-circle Kappa geometry goniometer for synchrotron use at the Swiss Norwegian Beam Lines at the ESRF in Grenoble.

In Oct 1999 a software project was launched to incorporate a modern instrument description and a user-friendly interface.

The poster will present the geometric model of the instrument based on the extension of a previous work [1]. The model is ready to accommodate point and/or area detector on the instrument. Furthermore some software features will be highlighted.

[1] Paciorek W. A., Meyer M., Chapuis G., On the geometry of a modern imaging diffractometer. *Acta Cryst.,* A55, pp.543-557, 1999.

s7.m0.p10 Comparison of optical elements for x-ray powder diffraction analysis in para-focusing and parallel beam geometries. C.A. Reiss, *Philips Analytical, Lelyweg 1, 7602 EA Almelo, The Netherlands.*
Keywords: X-ray powder diffraction, Bragg Brentano geometry, parallel beam geometry.

Structure determination from powder starts with a 'good' data set. For data collected on a laboratory instrument with a sealed tube the choice of optical elements and beam geometries has increased over the last years. The classical Bragg-Brentano para-focusing geometry is widely used but in the last decades parallel beam geometries are evolving rapidly. For both types of geometries an incident beam monochromator can be used to eliminate the $K\alpha_2$ radiation and as a result reduces peak overlap in the diffraction pattern.

For indexing a powder pattern it is important that the data is collected from a sample free of displacement error and is positioned exactly on the center of the goniometer in the Bragg-Brentano geometry. To be less sensitive for sample displacement one can use parallel beam geometry. Also for measuring transparent or irregularly shaped samples this geometry is the best choice. Parallel beam geometry can be realized by placing a narrow divergence slit or an X-ray mirror at the incident beam side of the diffractometer in combination with a parallel plate collimator at the diffracted beam side. When diffraction patterns become too complex the X-ray mirror can be replaced by a Hybrid monochromator. A Hybrid monochromator produces only $K\alpha_1$ radiation and has a resolution comparable to that of a high-resolution monochromator (about 25 arc seconds).

For samples that are sensitive to air, for small quantities, for transparent materials or for samples that exhibit shape texture a spinning capillary sample gives the best results in combination with an X-ray mirror or a Hybrid monochromator depending on the need for monochromatic radiation. On the diffracted beam side a position sensitive detector can be used to reduce data collection time.

Which optical element(s) and geometry are chosen for an experiment depend on the sample and the information that has to be extracted from the diffraction data. Often more than one measurement with different optical elements or beam geometries is needed to obtain the required data. Therefore the above mentioned configurations will be discussed and illustrated with measurements to show the advantages and disadvantages of the different optical components and geometries.