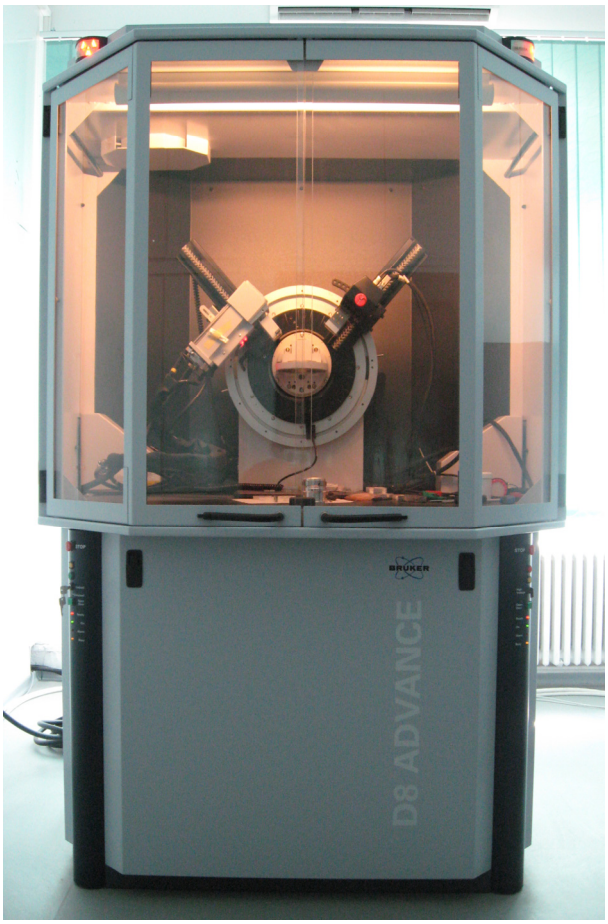
X-ray diffractometer, D8 ADVANCE type (BRUKER-AXS Germany, 2007)



X-ray diffractometer in powder XRD setting for structure analysis of polycrystalline and amorphous materials:

- qualitative and semi-quantitative phase analysis, lattice parameter and mean crystallite size determination (ICDD-PDF2 data-base, 2006 release);

- Rietveld structure refinement and quantitative phase analysis, structureless whole-pattern fitting according to Le Bail & Pawley (lattice parameters, crystallite size and strain), powder pattern indexing and ab-initio crystal structure determination.

Experimental setup:
- Vertical theta-theta goniometer in powder XRD setting; lowest step size (2θ)= 0.0002o; horizontal sample carrier;
nine-position multiple stage with automatic sample changer; fixed slit system.

- One-dimensional detector (LynxEye type) with collection rate about two orders of magnitude higher than that of conventional point detectors and very good angular resolution (default setting), or NaI(Tl) scintillation counter.
- Copper target X-ray tube used with nickel Kβ filter or with curved-graphite monochromator (default setting) or molybdenum target tube - if large scattering vector ranges are required.

Software:
- DIFFRACplus BASIC – software package for quick qualitative and semi-quantitative phase analyses, lattice parameter and mean crystallite size determinations; ICDD-PDF2 data-base, 2006 release;
- TOPAS 3.0 R/P/ I - software for: Rietveld structure refinement and quantitative phase analysis, structureless whole-pattern fitting according to Le Bail & Pawley (lattice parameters, crystallite size and strain), powder pattern indexing and space group determination and ab-initio crystal structure determination.