Universität Basel

Research Project

X-ray Diffractometer for Pair Distribution Function analysis of nanocrystals and nanostructured materials

Third-party funded project

Project title X-ray Diffractometer for Pair Distribution Function analysis of nanocrystals and nanostructured materials
Principal Investigator(s) De Roo, Jonathan ;
Co-Investigator(s) Constable, Edwin Charles ; Housecroft, Catherine ;
Organisation / Research unit
Departement Chemie / Nanomaterials (De Roo)
Department
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Nanoscience is at the frontier of research and is expected to provide new solutions in healthcare and energy. However, nanostructured materials in general and nanocrystals (NCs) in particular present a challenging problem: their structure is difficult to analyze with conventional techniques. Whereas powder X-ray diffraction (XRD) is very powerful for micron-sized crystals, extreme peak broadening precludes the accurate analysis of nanomaterials. As a consequence, structure-function relationships are hard to establish. Recently, a new technique has emerged, X-ray Pair Distribution Function (PDF) analysis, which allows to accurately model nanostructured materials. This requires a specialized diffractometer with high energy X-rays and a sensitive detection system. Many Swiss research groups are involved in nanostructured materials, including the main applicant, who was recently appointed as an assistant professor in nanomaterials with a research program featuring the synthesis and characterization of ceramic NCs. However, Switzerland does not yet have a PDF diffractometer available, hampering Swiss nanoscience. Therefore, we request here a PDF diffractometer with a silver source that yields the highest data quality possible for a lab diffractometer within a reasonable time (6 hours per sample).

With the requested diffractometer the main applicant will pursue several projects, both fundamental and applied. In the first three projects, the PDF method will be further improved by designing new PDF sample preparation techniques for colloidal NCs (increasing signal-to-noise and removing background scattering), implementing advanced modelling and integrating PDF with other analytical techniques. ăThis will greatly advance the use of lab source PDF diffractometers and establish PDF as a standard technique for NCs. In the second triad of projects, the main applicant will use PDF to support synthetic projects where the chemistry of (doped) metal oxide NCs is developed for bio-imaging applications and applied to shelling semiconductors NCs for solid state lighting applications. Together with the co-applicants and (inter)national collaborators, projects in the field of solar cells, photo-catalysis and thermoelectrics will be pursued. In these projects, the nanoparticle building blocks will be analyzed with the requested equipment and grant insight in their performance.ă

Keywords nanoparticles, nanocrystals, XRD, X-rays, Pair Distribution Function
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