'Physique et Chimie des Matériaux' – ED 397 – année 2020

PhD project for funding (max 1p), to send to

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Research unit (full name + acronym) : Laboratoire de Chimie de la Matière Condensée de Paris - LCMCP
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Keyword 1 : PDF Keyword 2 : Non Perfect Solids
Keyword 3 : Nanoparticle Keyword 4 : Defect
Select co-funding programme if applicable : select

Project title : Development of Pair Distribution Function for Non-Perfect Solids

Project Description (~4000 characters, font 11 min):

In order to build new advanced functional nanomaterials, the knowledge and understanding of the close relationship between atomic structure and property is essential. Nowadays, the elaboration of more and more complex materials require even more advanced characterization tools, especially at the local scale.

Pair Distribution Function (PDF) analysis provides such structural informations, when conventional X-ray Diffraction analysis is ineffective. The function G(r), representing interatomic distances distribution, is extracted from high quality diffraction data by ways of Fourier Transform and compared to the G(r) calculated as the probability of finding a pair of atoms at a distance r from a structural model. This approach particularly targets Non-Perfect Solids: ultrasmall nanoparticles, amorphous material, or material with crystallinity defects. Indeed, XRD copes with “imperfection” only via peak enlargement and increase of the background, meaning promotion of the perfect organization of a mean structure over the singularities of a real object. PDF analysis, at the contrary, takes into account all X-ray diffusive contributions and thus allows a more complete view of the material.

This PhD project propose to build new atomic models that will be confronted to experimental G(r) for validation. Three categories of materials that each represent a specific challenge have been selected. Synthesis of these materials have already been developed by LCMCP researchers.

(1) Ultrasmall nanoparticles. The reduced number of atoms (<6000) allows to build models with either independent atoms or stacked cells since such particles cannot be only described using cell periodicity.

Laboratory PDF analysis1 has already been performed on lanthanide oxysulfide highly anisotropic nanoparticle with tunable band gap. It was shown that sulfur ions were clearly lacking due to the strong anisotropy of the lamellar structure leading to non-stoichiometric solid. We now aim at building a complete model including the surrounding ligands usually used for limiting the particle growth, that will be validated though refinement.

(2) Doped nanomaterials. New algorithms are needed to detect the consequences of these defects on the surrounding atoms and distances.

Nb and W doped TiO2 nanoparticles, used in dye-sensitized solar cell setups to enhance charge collection efficiency of the photoanode, present the anatase structure2. We propose to use Differential PDF between undoped and doped particle to emphasize the effect of doping on the particles.

(3) Amorphous biomaterials. Several ways exist to describe an amorphous material: as a combination of a large number of different cells; as a crystalline material with various and numerous random defects or as a crystalline material presenting a very short range order. Bone mineral are composed of apatite nanoparticles surrounded by an amorphous layer. Related biomimetic materials have successfully been prepared and characterized3. The amorphous and crystalline phase will be investigated and compared to the crystalline/amorphous layer nanoparticles for comparison with the current model proposed in literature.

The successful construction of atomic models for these 3 kinds of samples which are representative of new advanced functional nanomaterials, will fulfill our PDF expertise. This will contribute to the construction of a database addressing the methodology to describe Non Perfect Solids for a better comprehension to the well-known structure properties relationship.

1 C. Larquet et al., Chem. Mater., 2019, 31, 5014–5023.
2 F. Dufour et al., Eur. J. Inorg. Chem., 2012, 2012, 2707–2715.
3 Y. Wang et al., Nat. Mater., 2013, 12, 1144–1153.