Poster Presentation

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Precession diffraction for reliable electron pair distribution function analysis

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Understanding and possible prediction of material physical properties depends upon the knowledge of the local atomic arrangement and crystal structure. Study of nanocrystalline or amorphous materials can be optimally performed with techniques like Pair Distribution Function (PDF) that is used to understand local atomic arrangement by using X-Ray, neutron or electron diffraction (ED) sources. ED related PDF (e-PDF) in Transmission Electron Microscope (TEM) has the advantage over X- Ray PDF technique that allows studying ordering of nanocrystalline materials in very local environment (nm scale instead of micron scale) by collecting (ED) patterns in very short time (ms instead of hours with conventional X-Ray Au or Mo sources). e-PDF has been recently applied to study nanoparticles [1] and amorphous materials [2] where is established that e-PDF match well equivalent X-Ray PDF. It was however observed that because of strong dynamical effects present in ED the height of such e-PDF peaks could become strongly altered in relation with theoretical calculated PDF peaks height. Although such dynamical effects do not affect accurate positions of e-PDF peaks that correspond to interatomic distances [2], they do have instead an influence on the PDF peaks height, and this can lead to wrong information on correct coordination number that corresponds to each e-PDF peak. In order to overcome this limitation for structure analysis, a theoretical calculation of the influence of dynamical ED scattering has been applied [2] on e-PDF for some materials with limited success. In our work we used precession electron diffraction (PED) where is known that its use decreases ED dynamical scattering [3] to study the influence on e-PDF analysis on NaYF4 nanoparticles. For our experimental work, a Libra 120 Kv microscope was used (IIT Pisa) with Digistar precession device (NanoMEGAS) and e-PDF commercial software (NanoMEGAS) based on [1]. We have observed that although the use of PED (or not) does not visibly affect ED NaYF4 patterns, it has on the contrary strong effect in the resulting e-PDF NaYF4 patterns where the long range order can be readily observed with PDF peaks height varying significantly with PED application (Fig1). In order to quantify precisely the PED influence on such e-PDF spectra we compared experimental calculation total area (obtained with and without precession) around the e-PDF peak at 2.36 Å (Na/Y- F bonding). Results shown on Table 1 below are very promising as show that use of Precession Electron Diffraction leads to very reliable information on the number of neighbours extracted from e-PDF peaks. Although our work was presently limited to NaYF4 nanoparticles , such results may encourage a more general use of PED tool for nanoparticles and disordered materials study in a TEM using e-PDF analysis.

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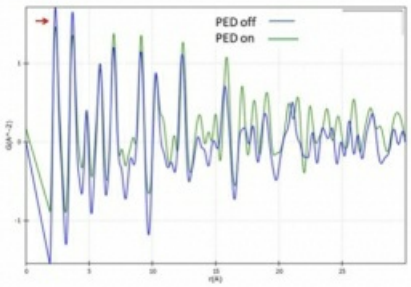

	Theoretical Coordination number (No of neighbours for hexagonal NaYF4 around Na/Y within 2.36 Å)	Experimental Coordination number (Area under the peak 2.36 Å)
No Precession	3	4.5
2 degree precession	3	2.9

Fig1 e-PDF calculated from ED pattern (with and without PED), arrow show peak at 2.36 Å.
Table 1 shows experimental (with and without PED) vs theoretical coordination number

Keywords: Electron Pair Distribution Function, Precession Electron Diffraction, Nanomaterials