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Solving ab-initio nanostructures with precession electron diffraction K. Boulahya[1], M. Parras[1], J. M. González Calbet[1] and S. Nicolopoulos[2,3] *[1]Departamento de Química Inorgánica, Facultad de Químicas, Universidad Complutense, E28040-Madrid, Spain. [2]Universidad Politécnica de Valencia/ITQ Avda de los Naranjos, Valencia 46071,Spain. [3]NanoMEGAS, Boulevard Edmond Machtens 79, Brussels B-1080, Belgium* E-mail: info@nanomegas.com

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Advanced materials structure analysis by electron diffraction in a transmission electron microscopy (TEM) presents a lot of advantages over conventional X-Ray diffraction: the size of studied crystallites in TEM can be very small, therefore individual phases in crystalline powders (nm size) can be examined. On the other hand, electron diffraction is much more sensitive than X-Ray as interaction with matter is many thousands times stronger in comparison. Again, in TEM, ED patterns can be obtained instantly with sufficient quality better than 0.05 nm resolution. Besides those advantages, electron diffraction has been used only scarcely for direct structure determination of nanocrystals [1]. The reason for this is that electron diffraction intensities can be strongly influenced by dynamical scattering effects that alter those intensities from ideal kinematical values and give rise to incorrect structure solutions in structure refinements, especially when ED data are taken from thicker part of nanocrystals.

However, today is generally believed that the precession electron diffraction technique developed by Vincent and Midgley in 1994 [2], is the most promising method for reducing dynamical effects in diffraction patterns and collecting a suitable set of reflection intensities suitable for structure determination. In the precession method, the crystal is first oriented along a zone axis, then, by using the upper TEM scan coils, the beam is tilted and precessed around the optical axis on a conical surface [2]. The electron beam is then descanned in such way that a stationary spot diffraction pattern is obtained (for precession frequencies > 1 Hz). Due to this geometry, electron diffraction pattern consists of many reflections far out in reciprocal space with intensities that are integrated over the excitation error.

In this work, we present results obtained for several heavy atoms oxide compounds using precession electron diffraction (PED) data to solve the structure.

[1] ICCD Inorganic crystal structure (ICSD) ver: 2005– Factinformationscentrum Karsluhe and US Dept of Commerce.
[2] R Vincent, P.A Midgley, *Ultramicroscopy* 53 (1994) 271