Im2Cr: An efficient tool for crystallographic indexing of HR(S)TEM images

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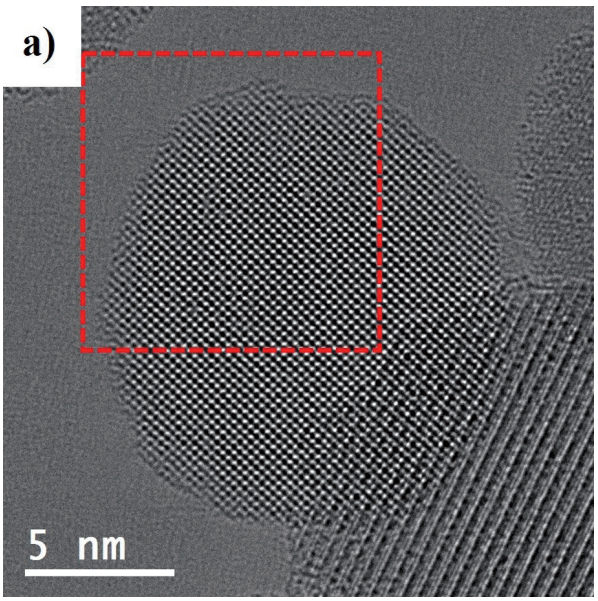
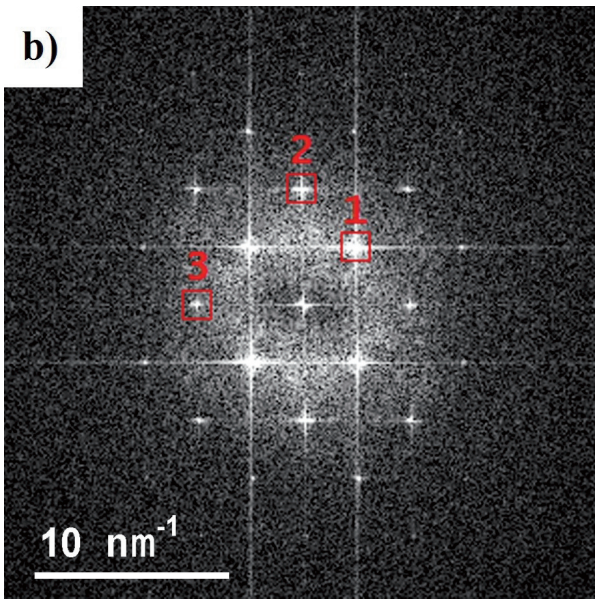
Transmission Electron Microscopy (TEM) and Scanning TEM (STEM) have been widely used to characterize nanostructured materials with atomic resolution, and significant advances on their experimental setup greatly extended the current pool of analysis possibilities at the nanoscale. The exploration of advanced (S)TEM characterization capabilities and their reproducible application to reach a suitable sampling is often restricted by the extensive data analysis procedures required to reliably interpret experimental results and to extract quantitative information. Even routine tasks such as nanoparticles crystallographic indexing from electron diffraction patterns or from high resolution (S)TEM images are mostly carried out manually by the users, resulting in a reduced TEM characterization yield and significant user bias.

This work presents Im2Cr, a new software tool to aid the crystallographic indexing of nanostructured materials using high resolution (S)TEM images. Im2Cr implementation aims for a minimal user interaction, supporting the detection of zone-axis oriented particles, and including an efficient peak detection process applied to the images Fourier Transform (FT). With basis on the FT peaks distances and relative angles, crystallographic indexation is carried out autonomously via comparison with a list of candidate structures named by the user, and a ranking of the best matching combinations of crystallographic structures and viewing zone axes is generated.

Im2Cr was successfully tested for robustness and execution efficiency in a wide range of High Resolution (S)TEM images from crystalline nanomaterials, with domain size ranging from 4 to 100 nm. The autonomous indexation with preset parameters has a very high success rate, and runs in a small fraction of typical (S)TEM images acquisition time by taking advantage of the inherent hardware parallelism. Alternatively, the user can operate Im2Cr in a semi-autonomous mode and control relevant parameters related to the region of interest (ROI) selection on the (S)TEM image and on the FT peaks detection. Im2Cr promising results point to the possibility of real-time image analysis with reduced user interaction, allowing for an increased (S)TEM characterization yield and also enabling the interpretation of complex images, such as those from nanocrystalline materials imaged in high-order zone axis orientations.



a) Fe3O4 nanocrystal HRTEM image obtained at 200kV using a NCSI(1) imaging setup. The inset (red square) indicates the selected ROI.
(1) - Urban, K. et al. Phil. Trans. R. Soc. A 367, 2009, 3735-3753.



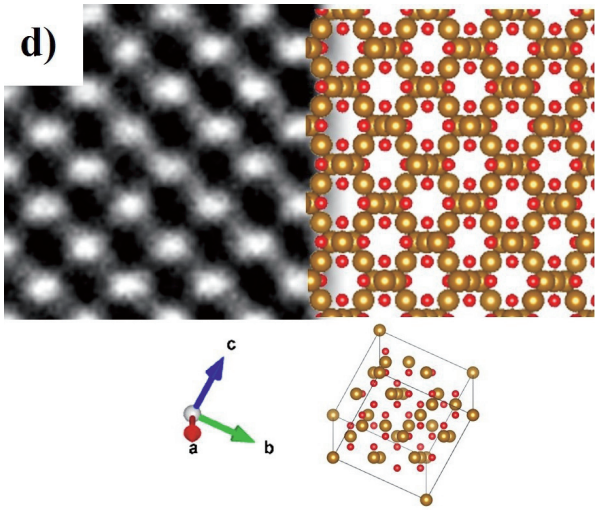
b) FT from the ROI region and the detected peaks related to the crystalline structure.

c)

Experimental results		
Spots	Distance (nm)	Angle (degrees)
1	0.256	0
2	0.170	43.7
3	0.185	132.5

Index with reference CIF (Fe_3O_4 - #1011032)			
Spots	Index	Ref. distance	Ref. angle
1	{ 1 -1 -3 }	0.251	0
2	{ 2 2 -4 }	0.170	42.4
3	{ 0 4 2 }	0.186	132.5
Match (%)	**Zone Axis**	**Upward vector**	
95.83	<5,-1,2>	[1.9955 2.0045 -3.9865]	

c) Crystallographic indexing results, including the best matching crystallographic information file (Fe3O4 - #1011032) among the listed candidates (Fe3O4 - #1011032; FeO - #1011169; Fe2O3 - # 1011267), the FT spots indexing and their overall match, the viewing zone axis and upward vector.



d) Comparison of the HRTEM image detail and < 5 -1 2 > zone-axis oriented Fe3O4 crystalline structure(2). The akin periodicities indicate a correct crystallographic indexing.
(2) - Momma, K.; Izumi, F.; J. Appl. Crystallogr. 44, 2011, 1272-1276.