Inversion detection in $CoFe_2O_4$ spinels by EELS and A-BM3D analysis

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In the domain of catalysis and gas sensing, the size, shape and composition of ferrite nanoparticles can be tuned to adjust their properties [1]. In order to tailor the reactivity and catalytic properties of cobalt ferrites, nano-ferrites with different shapes, e.g. nano-octahedra and nanocubes, can be synthesized using solvothermal methods for which the shape of nanoparticles is governed by the differences in growth velocity of specific crystallographic facets, which in turn can be controlled by the use of specific surfactants. Cobalt ferrites are mixed ferrites, with an inversion degree that varies with the cobalt content, particle size and the synthesis method, so the cation distribution about the tetrahedral and octahedral sites, should also be considered when discussing cobalt ferrite properties.

Here we apply A-BM3D analysis to the problem of mapping the Co Fe and O distributions in nanocubes with a view ultimately to measuring the inversion parameter. The main challenge in performing the experiment arises from the beam-sensitive nature of the material, meaning that only hyperspectral with quite poor statistics can be acquired before the damage becomes significant.

Principal components analysis (PCA) is a dimensionality reduction method often used in EELS to perform denoising of the data [2] by reconstructing the spectrum image (SI) by keeping only the most significant components, the others being interpreted as noise. However, this method has the disadvantage of not taking into account the spatial correlations present in the hyperspectral image. Indeed, for our data the elemental maps obtained by this method remain quite noisy.
Denoising algorithms considering jointly the spatial and spectral correlations are more promising in terms of performance. We have used a sequential approach associating dimensionality reduction by PCA with spatial denoising of component weight maps. Map denoising is performed by the standard version of Block matching and 3D filtering (BM3D, a patch method) which is one of the best performing 2D image denoising algorithm [3]. This algorithm requires an estimation of the noise variance. A-BM3D, as a sequential method, has the advantage of being of limited complexity compared to joint methods that operate directly on the spatial/spectral cube.
Once the SI is denoised, the chemical maps are obtained by the classical method of background subtraction and integration of the characteristic signal. Initial estimations based on the spot intensities in the maps give an inversion parameter $x = 0.75 \pm 0.2$. Further work is needed to refine this figure.

Using A-BM3D is seen to improve significantly on conventional mapping and denoising using PCA.

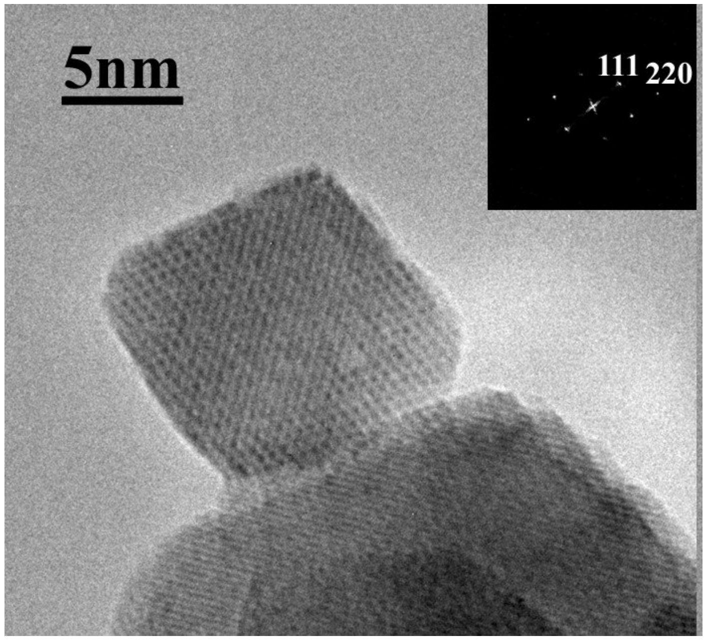

Figure 1. HRTEM image of typical $CoFe_2O_4$ nano-octahedrons

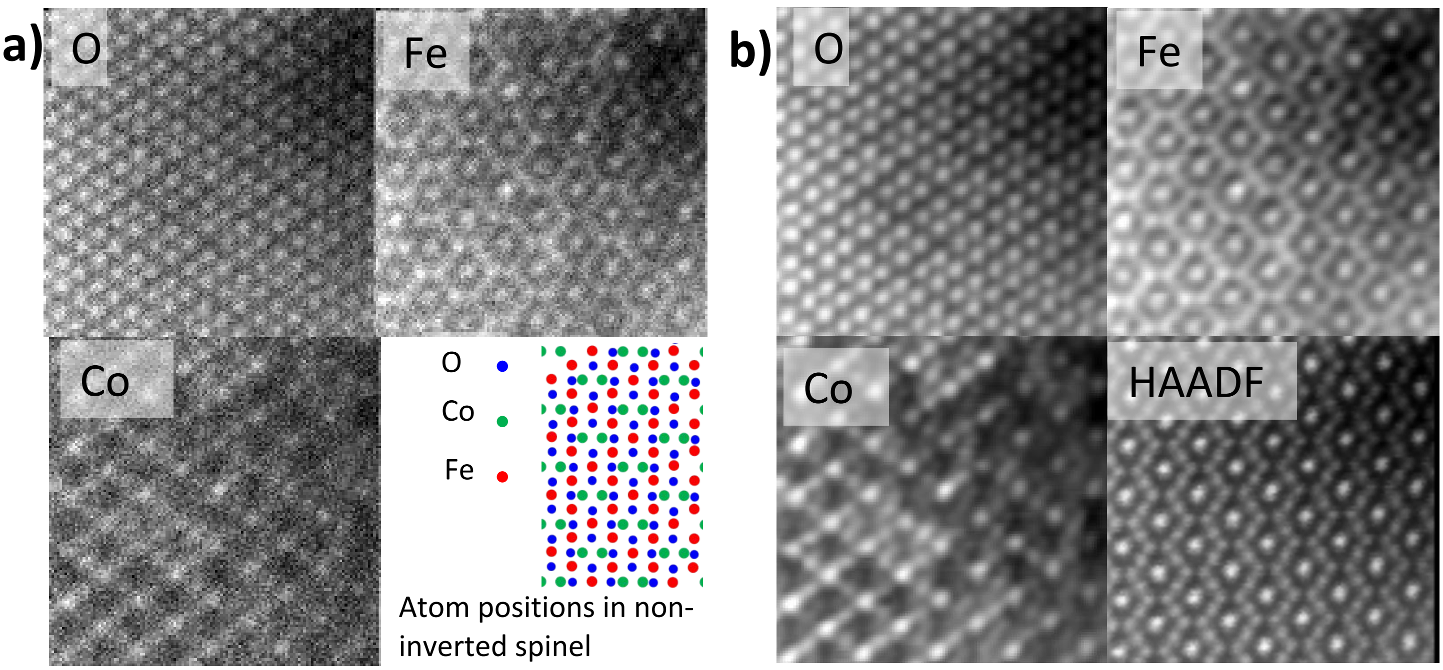

Figure 2. EELS Elemental maps in the [110] direction after a) PCA and b) PCA+BM3D. Also shown are the atomic position projections in the non-inverted spinel and the simultaneous HAADF image.

References

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[4] We thank ESTEEM3 (Europe), METSA (France) and the “Equipex” project TEMPOS (France) for financial support.