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Aberration Correction and Exit Wave Reconstruction of Metal and metal Oxide Nanoparticles.

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Abstract – The combination of electron optical aberration correction and exit wave reconstruction has been used to provide detailed structural information about the surface structures of both metal and metal oxide nanoparticles for direct comparison with quantitative phase diagrams constructed using multiscale thermodynamic models.

Electron optical aberration correction in both TEM and STEM geometries is established [1,2] with a variety of imaging and probe corrected instruments installed at many laboratories around the world.
An alternative, complementary approach to direct correction involves computational compensation of measured coefficients of the wave aberration function, *a posteriori* during exit wave reconstruction from series of images recorded with different focus values [3], or with different illumination tilts [4]. The former extends the interpretable resolution to the axial information limit [3] and has been applied to aberration corrected images [5]. However, the latter provides information beyond the axial information limit of the microscope [4]. For corrected instruments computational reconstruction is beneficial in both geometries as it compensates for higher order aberrations, which cannot currently be directly corrected. It can also be used to locally refine the residual lower order aberrations as a function of image space. Exit wave reconstruction also gives access to complex data set not obtainable from a single image. In the characterisation of nanoparticles this additional data provides key information about local surface structures that can be directly compared with quantitative phase diagrams constructed as a function of particle size for a wide temperature range.

Figure 1 illustrates the cumulative effects of initial direct electron optical correction followed by subsequent aberration refinement on data obtained from a nanocrystalline Pt catalyst particle demonstrating the improvement obtained by recovering the specimen exit wavefunction compared to the information present in a single HRTEM image. In particular local atomic steps and terraces on the {111} surfaces are clearly visible in the reconstructed phase and these have a direct bearing on the catalytic activity of these particles. In the case of oxide nanoparticles specific surface terminations can be directly observed which enables a prediction of the redox behavior of these species. Finally, recent instrumental developments have enabled atomic resolution data to be recorded as a function of temperature enabling the behaviour of these systems under catalytically relevant operating conditions to be investigated.

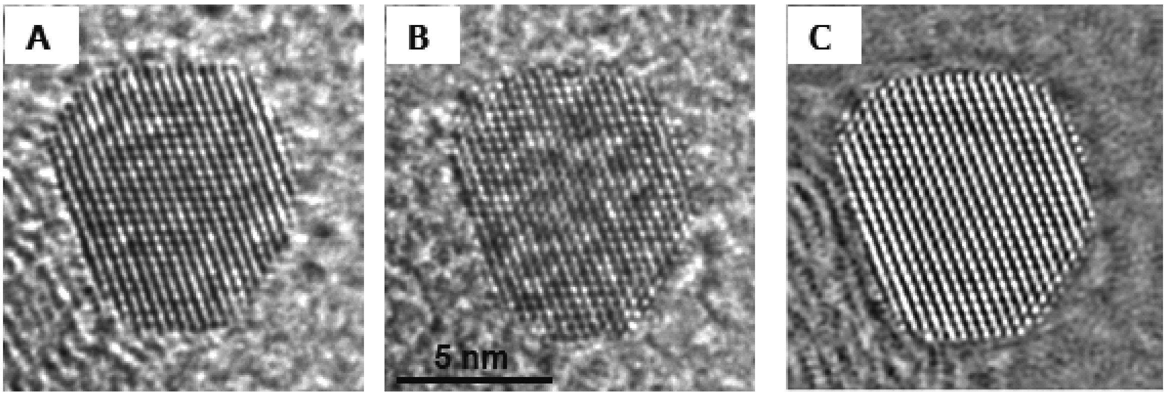

Figure 1: Figure 3 (a, b) HRTEM (intensity) images of a nanocrystalline Pt catalyst particle acquired with C_S uncorrected at 0.5 mm (a) and corrected to -30 μm (b). (c) Phase of the specimen exit plane wavefunction of the same particle, obtained after aberration compensation and refinement of a through-focus series of aberration-corrected images

References

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