method to determine the surface crystallography of single crystal gold nanorods grown in the presence of Ag and found that, contrary to the current consensus, the surface facets are sparsely packed atomic planes [2]. This result has profound implications for understanding nanocrystal growth and morphology and forces a reconsideration of established theoretical models of nanoparticle growth.

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Keywords: quantitative scanning transmission electron microscopy, thickness profile determination, gold nanorods morphology.

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Real space charge density mapping by quantitative convergent beam electron diffraction (QCBED)

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Quantitative energy-filtered convergent beam electron diffraction (QCBED) can be used to measure the low order structure factor amplitudes and phases of microcrystals of known structure very accurately. This TEM-based technique uses a small electron probe of nanometer dimensions, so that a perfect crystal region can be selected for electron diffraction. It refines structure factors, absorption and specimen thickness using multiple scattering calculations, and measures the structure factors on absolute scale. Thus, extinction corrections, absorption corrections and scaling problems are avoided in electron diffraction. For non-centrosymmetric crystals, the refinement of charge density maps requires highly accurate measurements of structure factor phases, which can now also be measured using the QCBED method [1-3]. Electron diffraction is much more sensitive to ionicity at low scattering angles than X-ray diffraction [3], making it more suitable for charge-density mapping and the imaging of bonds. The accuracy is equivalent to that of the X-ray Pendullösung method [4-5], allowing the covalent and ionic contributions to be separately visualised.

Accurate structure factors of Cu, GaN and AlN have been measured by QCBED. The measurement standard deviations are normally less than 0.2% for both amplitudes and phases of low order structure factors. Accurate charge density maps have been obtained and the bonding character has been studied. Multipole refinement on Cu supports a free electron model [5]. Polar covalent bonds in Ga-N and, Al-N are observed in experimental charge density maps, using multipole refinement of combined measurements of structure factor magnitudes and phases [1-2].

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Keywords: quantitative convergent beam electron diffraction (QCBED), real space charge density, bonding

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Direct measurements of lattice distortion and mapping of point defects

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Recent advances in transmission electron microscopes (TEM) have enabled detection of light atoms, even the lightest hydrogen atomic columns, which have scattering strength too weak to be detected by non-aberration corrected TEM.[1] The detection limit of the state-of-the-art TEM/scanning TEM (STEM) has been tested in diverse systems; for example, identifying single light atom such as nitrogen and boron, and probing charge redistribution by chemical bonding [2-3]. Image simulations in those reports were essential to verify the experimental results. In fact, low signal to noise ratio in extreme measurements often requires substantial data processing as well as significant amount of experimental data.

Here, we present image and diffraction simulations to access the feasibility of detecting structural defects in a crystal such as point defects and static displacements. It is well known that local strain fields by structural defects enhance contrast in images. We exploited first-principles calculations to find relaxed structures of a crystal with point vacancies as well as a crystal with a structural distortion caused by strain in complex oxides. The multislice method was employed to simulate STEM images and convergent beam electron diffraction patterns of both the relaxed structures and non-relaxed structures. Adjusted parameters include convergence angles, focal depths, and scattering angles. Furthermore, the contribution of bonding charges to the images was examined by comparing simulation results using projected potentials from the first-principles calculations and using conventionally used atomic potentials.

Image simulations on strained oxide materials with tetragonal distortion, such as $NdNiO_3$, were applied for structural analysis. We used an aberration corrected microscope for atomic-resolution STEM images, and performed quantitative analysis of the image to extract structural parameters. The results were compared with the first-principles calculations, which indicated reliability of this approach.

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Vapour induced transformations investigated by powder diffraction analysis

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Solvent vapour exposure on the organic crystalline materials often induces pseudo-polymorphic transformations (solvation, solvent exchange and desolvation). Such transformations have potential to improve and/or control the solid-state properties of the target materials and are important phenomena in the field of material science. However, such transformations have not been completely understood because of