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Visible and Invisible in Aberration Corrected STEM: A Comparative Survey of Theory and Experiment

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VISIBLE AND INVISIBLE IN ABERRATION CORRECTED STEM: A COMPARITIVE SURVEY OF THEORY AND EXPERIMENT

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ABSTRACT: The increasing availability of aberration correctors [1] for scanning transmission electron microscopy (STEM) is bringing substantial improvements in sensitivity. As the features being resolved have approached the atomic scale, the importance of dynamical channelling in the image formation process has also increased. Many authors have noted the potential for ambiguous interpretation and have stressed the need for theoretical simulations as part of the process of interpreting experimental results [2-4]. Recently, a theory has been presented for the use of the so-called mixed dynamical form factors (MDFF) which allows simulation of HAADF and EELS images using either Bloch wave or multislice methods [4].

The 100 kV VG Microscopes' HB501UX at Oak Ridge National Laboratory, equipped with a Nion aberration-corrector, now routinely provides resolution close to 1 Å. With this microscope, *single atom* spectroscopy has been achieved [5] for La-doped CaTiO₃. The 300 kV VG Microscopes' HB603U STEM at Oak Ridge National Laboratory, also fitted with a Nion aberration-corrector, is producing a probe of 0.7 Å diameter. The increased sensitivity has also allowed O columns to be imaged at an α -Al₂O₃/SrTiO₃ interface and is providing considerable insight into the structure of interface layers in Si₃N₄.

This talk will give an overview of these results with particular reference to the corresponding simulations. The simulations predict the visibility of oxygen in SrTiO₃, and are particularly important to demonstrate that it is the oxygen columns which are contributing to the HAADF image, rather than adjacent, heavier columns as a result of the channelling. The prospects for seeing atoms lighter than oxygen are discussed.

Contrast from single atoms in a zone-axis crystal is complicated by depth-dependent dynamical behaviour of the wave function. We demonstrate this effect through simulations of single atom spectroscopy images of La-doped CaTiO₃. We present simulations and describe the issues involved in accounting for the contribution measured on adjacent columns.

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