Imaging Point Defects in Complex Oxides Using Quantitative STEM

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While methods to measure the global concentration of point defects exist, determining their spatial arrangement is significantly more challenging. Furthermore, most techniques cannot provide direct information about atom relaxations around a point defect even though these are crucial for many properties. HAADF-STEM images can provide three-dimensional information of the location of individual dopant atoms in $SrTiO_3$ from a *single image*. The contrast and interpretability can be improved using *variable-angle HAADF-STEM* (VA-HAADF). Detecting *vacancies* in STEM images is even more challenging than dopant atoms that have a large atomic number difference with the host. We have combined VA-HAADF and rigid registration methods to detect Sr vacancies in $SrTiO_3$ *and* their associated local atom relaxations. Lattice relaxation around the vacancies are detected with picometer precision. Rigid registration methods not only improve the precision in measurements of atom column positions but also the quantification of image intensities, which allows for the detection of point defects with low Z-contrast, such as vacancies. We also investigate atomic-scale structural relaxations upon doping a prototype Mott insulating material, $SmTiO_3$, with Sr. As the Sr content increases, the orthorhombic distortions gradually decrease. Measurements of the atomic column positions provide direct evidence of continuous and homogeneous structural changes with no signs of phase separation. The detailed structural information with high spatial resolution and precision and provides an important step toward a complete understanding of unconventional physical phenomena near Mott transitions.