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Progress in Applications of Quantitative STEM

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High-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) is highly sensitive to the type and number of atoms in the atomic columns of a sample. Image contrast in HAADF-STEM agrees quantitatively with image simulations [1]. An important complementary method in STEM is position averaged convergent beam electron diffraction (PACBED), which is highly sensitive to information that cannot easily be obtained from HAADF-STEM images, such as small displacements of atom or tilts of oxygen octahedra in perovskite materials [2, 3]. In this presentation, we will discuss our recent [4, 5] work in applications of quantitative HAADF-STEM and PACBED to pertinent problems in materials science.

Our first example concerns the determination of the three-dimensional location of individual Gd dopant atoms in SrTiO3 [4]. The method is based on using quantitative comparisons of experimental and calculated image intensities. Quantitative measures of the error and a criterion for the dopant visibility were established using an undoped SrTiO3 sample. The overall dopant concentration measured from atom column intensities agrees quantitatively with Hall carrier density measurements. The method is applied to analyze the 3D arrangement of dopants within small clusters containing 4-5 Gd atoms (Fig. 1).

Our second example discusses the correlation between oxygen octahedral tilts, A-site cation displacements, and ferromagnetism in thin, confined GdTiO3 layers. We show that PACBED in combination with HAADF-STEM imaging can be used to obtain independent information on tilts and displacements (Fig. 2) [5]. With decreasing GdTiO3 film thickness, structural distortions are reduced, concomitant with a reduction in the Curie temperature. Ferromagnetism persists to smaller deviations from the cubic perovskite structure than is the case for the bulk rare earth titanates, which allows for insights into strong electron correlation physics.

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(a) (b)

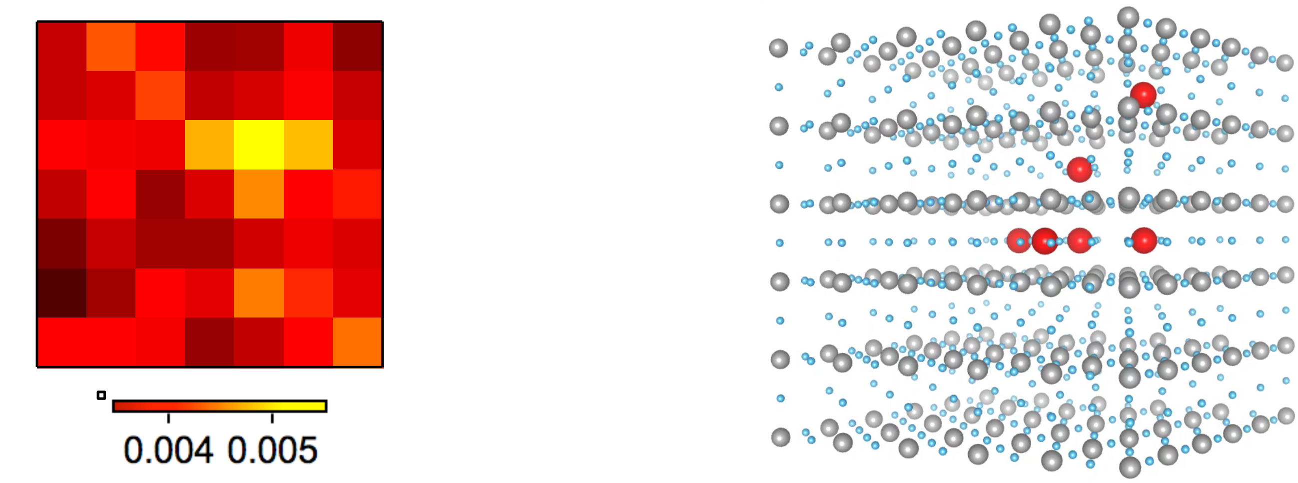

Figure 1. (a) Quantitative Sr column intensity map from a Gd-doped $SrTiO_3$ foil, from which the 3D Gd dopant atom (shown in red) configuration shown in (b) was determined. From ref. [4].

a) (b)

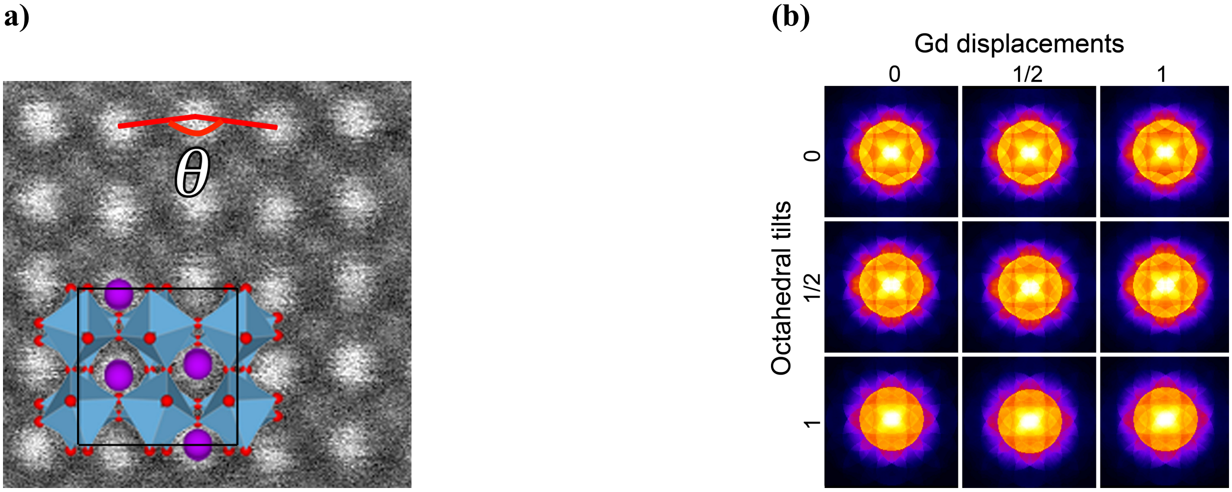

Figure 2. (a) Quantifying Gd-displacements in a confined $GdTiO_3$ film. (b) Simulations that show that PACBED is sensitive the Ti-O octahedra tilts but not to Gd displacements, thereby providing complementary information to the images. From ref. [5].

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