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Application of Aberration Corrected Scanning Transmission Electron Microscopy to the Study of Interfaces and Defects

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In addition to improving the spatial resolution, aberration correctors have greatly improved the sensitivity of Z-contrast images in the scanning transmission electron microscope (STEM). The ability now exists to directly correlate atomic scale changes in composition with the structure of nanostructures, interfaces and defects, leading to a much better understanding of the origin of materials properties. However, these desirable advanced capabilities are accompanied by a potentially problematic increase in beam current, so that if the experiment is performed using the same methodology as conventional imaging, the sample is much more susceptible to beam damage effects. To mitigate the effect of beam damage, the well established methods of low-dose imaging, image processing and structural averaging used in the biological sciences can easily be employed.

One example where such methods can be utilized is in the analysis of the incorporation of N into GaAs to form a GaAsN alloy. These alloys have important applications in the optoelectronics industry where the potential applications depend on the ability to incorporate N in the structure without forming defects. The low-resolution Z-contrast images in figure 1 show that there is a surprising effect of GaAsN alloy formation. Despite the lower atomic number of N, the layers with higher N concentration are brighter. By using the aberration corrector to obtain atomic resolution images of the structures, correcting for thickness variations and averaging over large areas of the image to obtain statistically significant contrast variations, the origin of the contrast can be determined to be due to the distortion of the lattice by the incorporation of the smaller N atoms. Furthermore, the contrast variability and the shape of the GaAs dumbbells in the image allow the particular point defect complex to be identified from the 4 possible structures predicted by density functional theory.

Another application is the study of low-angle grain boundaries in $SrTiO_3$. Studies of grain boundaries in $SrTiO_3$ have focused on the assignment of structural units that represent the atomic structure of the dislocation cores. However, recent analysis of a series of ~200 Z-contrast images (Figure 2) obtained in an aberration corrected STEM have shown that there can be significant variability in the atomic positions in these units (on a sub-unit cell scale). By statistical analysis of all the images, the most likely structure, and variability of the atomic locations can be mapped directly (Figure 2). In this case, the center of the core maps out the favorable low-energy positions of the atoms as a function of the strain and composition distribution – which can be directly compared with the low-energy structures obtained by DFT.

In addition, the modified experimental methods can be used to study highly mobile nanoparticles, organic materials and to extend the precision of structures determined from experimental images [1].

References

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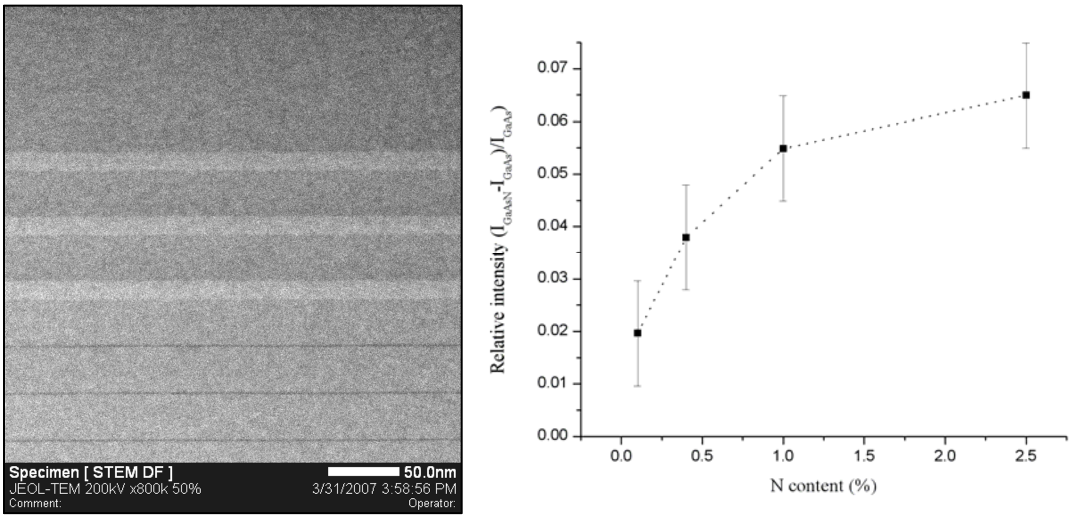

FIG. 1. (a) Low magnification HAADF-STEM images of the GaAsN quantum wells with 2.5%N. (b) Plot of the evolution of contrast with N content from a series of GaAsN Quantum wells.

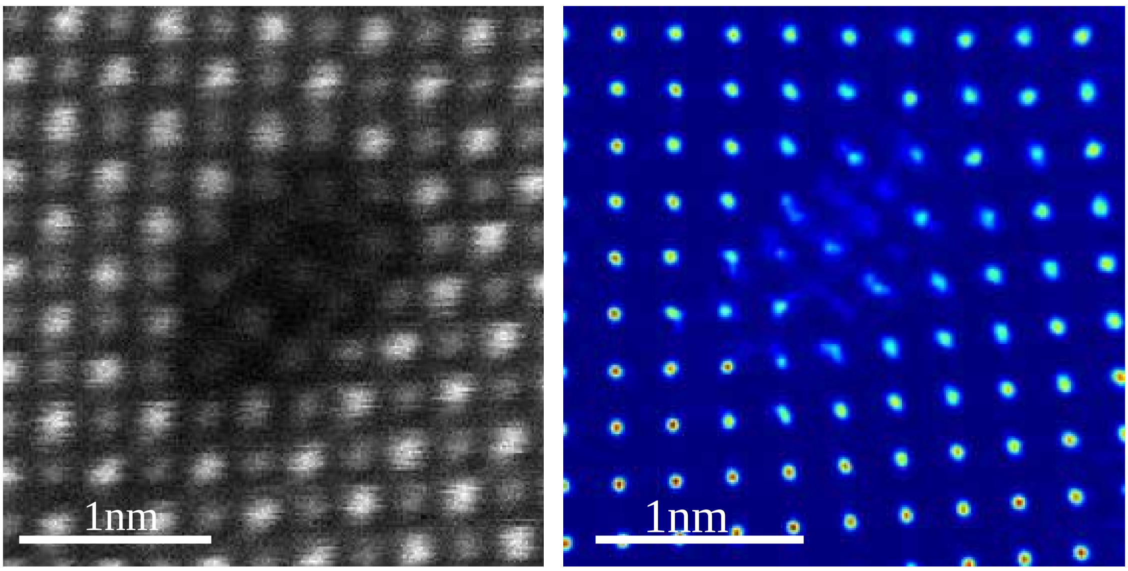

FIG. 2. (a)Representative Z-contrast image of a dislocation core in a low-angle $SrTiO_3$ grain boundary. (b) Probability distribution of atom locations based on images of ~200 cores.