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Invited talk at the 8th Conference on Frontiers of Electron Microscopy in Materials Science, National Research Institute for Metals, Matsue, Japan, November 16, 2000.

STRUCTURE-PROPERTY RELATIONS FOR INTERFACES AND NANOSTRUCTURES THROUGH Z-CONTRAST IMAGING, EELS AND THEORY

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Prepared by the

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Under Contract DE-AC05-00OR22725

October 2001

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In the aberration corrected STEM the ultimate resolution for a zone axis crystal will become not the probe, as in the case of isolated atoms, but the 1s Bloch states. In fact, the *Z*-contrast image becomes a direct image of the 1s Bloch states with limiting intensities for large thicknesses roughly proportional to Z^2. Not only resolution but image contrast and signal to noise ratio will improve dramatically. EELS is sufficiently localized to see similar advantages. In the limit of a large collector aperture, the delocaliztion of core loss EELS is just the size of the core electron orbital itself.

Together with first-principles theory, it is possible to obtain a deep insight into the atomistic origin of materials properties. In the case of $SrTiO_3$ grain boundaries, the origin of the electrical activity has been shown to be due to oxygen deficiency that leads to undercoordinated cations and band bending. The same effect explains the exponential reduction in critical current at grain boundaries in YBCO. Provided the effects of core excitons are included, the same theoretical methods provide a quantitative simulation of EELS core loss fine structure, enabling experimental spectra to be inverted, and showing the importance of interfacial bonding for the electronic properties of the Si/SiO_2 interface.