

Spectral Imaging of the EELS Spectra Using *ab initio* Data and Function Field Visualization

Paul Rulis and W.Y. Ching

Department of Physics, University of Missouri-Kansas City, Kansas City, Missouri 64110 USA

Electron energy-loss spectroscopy (EELS) in conjunction with high resolution scanning transmission electron microscopy (STEM) with sub-angstrom atomic resolution has been an effective characterization tool for imaging materials. Recent instrumentation developments, such as aberration correction (AC), and related data processing techniques have pushed spectral imaging (SI) to an unprecedented level of sophistication [1]. However, many technical challenges still remain. On the other hand, multi-dimensional data visualization techniques have become significantly more powerful over the past few decades. A relatively new area of development concerns function fields [2]. Here, each point in space is associated with a one dimensional function which may be represented by some correlation value such as total area of spectrum within an energy window, energy-loss peak or ELNES edge on-set. In this approach, a single function from the set of functions is chosen as a target, and all the functions from the other spatial points are compared to the target using a weighted Euclidian difference. The scalar value at each point then represents the dissimilarity between the function at that point and the target point. Since the difference can be weighted, it is possible to emphasize particular parts of the function for the purpose of feature identification.

We show that by using accurate data obtained from *ab initio* calculations of atom-specific absorption edges and by incorporating function field visualization, much insight regarding the effects of interatomic interaction on the spectral images can be obtained, making it a potentially a powerful tool for direct imaging of microstructures and defective materials. We present the results of applying this approach to two systems as examples: (1) The symmetric 53° $\langle 001 \rangle$ tilt $\Sigma = 5$ grain boundary in SrTiO₃ which contains buckled Sr columns and an alternating Ti-O columns in the $\langle 001 \rangle$ projection [3,4]; and (2) the planar {113} extended defect model in crystalline Si with 8-, 7-, 6-, and 5-member rings and no dangling bonds [5,6]. The Sr-K, Ti-K, O-K and Si-K and Si-L₃ edges of every single atom in these models were calculated using the supercell OLCAO method [7] to accumulate the *ab initio* data for SI. Some of these results are illustrated in Fig. 1 and Fig. 2 respectively.

In summary, we suggest a new approach to spectral imaging by *using ab initio* data calculated theoretically combined with functional field visualization technique.

References

- [1] C. Colliex, Nature 450, 622-623 (2007).
- [2] J. C. Anderson, L.J. Gosink, M.A. Duchaineau, and K.I. Joy, Eurographics/IEEE-VGTC Symposium of Visualization, ed. K. Museth, T. Moller, and A. Ynnerman, (2007).
- [3] M. M. McGibbon, N.D. Browning, M.F. Chisholm, A.J. McGibbon, S.J. Penneycook, V. Ravikumar, and V.P. Dravid, Science 266, 102 (1994).
- [4] S. D. Mo, W.Y. Ching, M.F. Chisholm and G. Duscher, Phys. Rev. B60, 2416 (1999).
- [5] H. Kohno, T. Mabushi, S. Takeda, M. Kohyama, M. Terauchi and M. Tanaka, Phys. Rev. B58, 10338-342 (1998).
- [6] Y. Chen, S.-D. Mo, M. Kohyama, H. Kohno, S. Takeda, and W.Y. Ching, Materials Trans. 43 (7), 1430-1434 (2002).
- [7] S. D. Mo and W.Y. Ching, Phys. Rev. B62, 7901-7907 (2000).

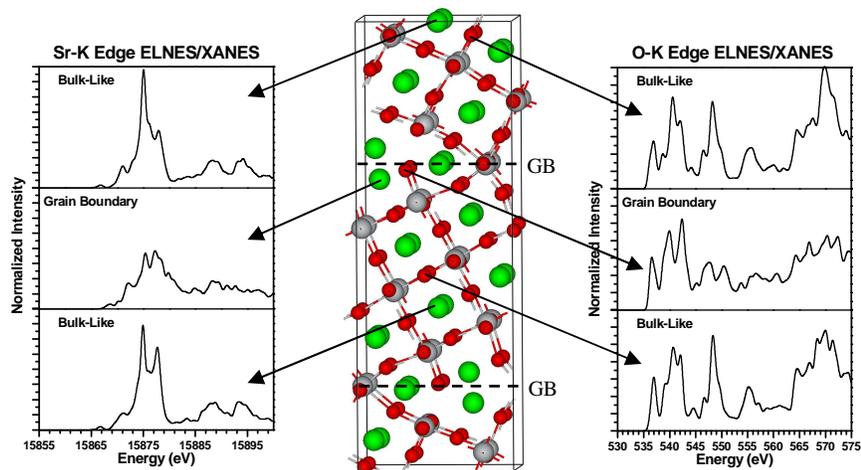


FIG. 1: The calculated Sr-K and O-K edges for atoms from different regions of the $\Sigma = 5$ grain boundary (GB) model in SrTiO_3 . Note that there are two oppositely oriented GBs in this periodic model.

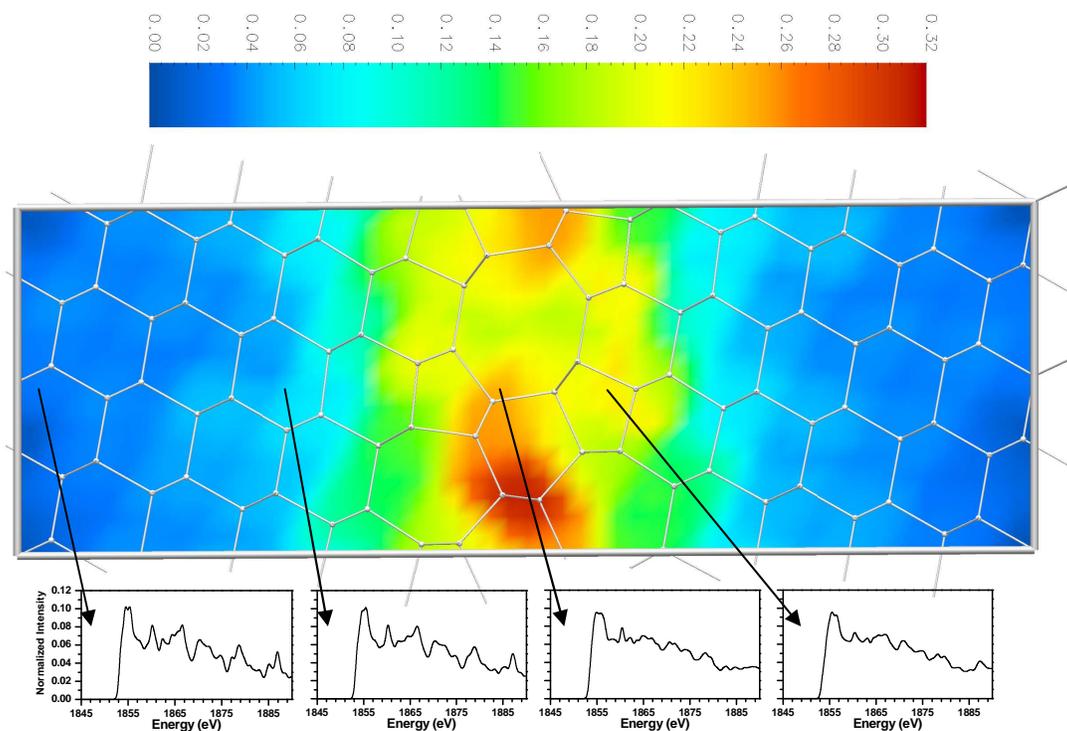


FIG. 2: Spectral image (SI) showing the deviation of the Si-K edges (in the first 40 eV range) from that in the bulk Si region in the planar $\{113\}$ defect model. The plane shown here is perpendicular to the $\langle 110 \rangle$ direction. The image data, which are obtained on a three dimensional mesh averaged over the $\langle 110 \rangle$ direction, contain information about the Si-Si inter-atomic bonding in a passive defect. The thin white lines show the bonds between Si atoms and the ring structure. The four lower panels show the first 40 eV of the Si-K edge from four different locations.