acutely sensitive to local site symmetry. Furthermore, these inelastic images illustrate the complex nature of the scattering from the boron octahedra. The implications for extracting information about individual atoms within a specimen using conventional quantitative STEM and using direct images of the scattered electron probe will be discussed.

[1] K. Ishizuka, *J. Electron Microsc*. **2001**, *50*, 291-305. [2] C. Dwyer, J. Etheridge, *Ultramicroscopy* **2003,** *96*, 343-360. [3] C.J. Rossouw, L.J. Allen, S.D. Findlay, M.P. Oxley, *Ultramicroscopy* **2003,** *96,* 299-312. [4] P. Voyles, Grazul, D.A. Muller *Ultramicroscopy* **2003** *96***,** 251. [5] J. Etheridge, S. Lazar, C. Dwyer, G.A. Botton, *Phys Rev. Lett* **2011,** *106*, 160802.

Keywords: scanning transmission electron microscopy, electron scattering, double-aberration correction.

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***QFocus*: Structure reconstruction from focal series of hrtem images**

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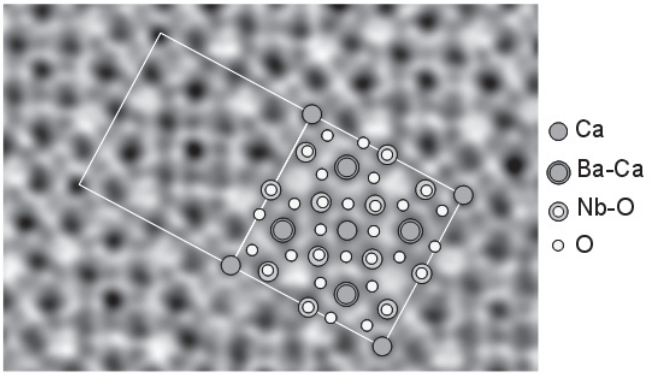
High-resolution transmission electron microscopy (HRTEM) images are usually not directly interpretable in terms of crystal structure due to various aberrations in the microscope lenses. Although significant progress has been made recently in the development of hardware aberration correctors, especially spherical-aberration correctors [1], the majority of transmission electron microscopes in use today are traditional ones and structure reconstruction by software methods still serves as a cost-effective alternative. Representative software methods include exit wave reconstruction using through-focus image series [2] and contrast transfer function (CTF) correction methods using single images or image series [3]. Here we present a CTF-correction based structure reconstruction method, using through-focus series of HRTEM images taken with a fixed focus step, in which all images in the series are corrected for CTFs and combined into a structure image. To determine the starting defocus of the series, trial defocus values in a large range are tested and CTF corrections are made to all images. The similarity of the phases of the Fourier transform between the corrected images is used as the criterion to judge whether a trial defocus value is close to the true one. The two-fold astigmatism is determined by dividing Fourier transforms into sectors and determining the defocus along different directions. As crystallographic phases are used in defocus and astigmatism determination, no amorphous areas are required in the images. On the other hand, since CTF correction is done for all pixels within the resolution limit in reciprocal space, this method works for both perfect and defect crystals.

The method was applied on a 20-image focal series of $Ca_{0.28}Ba_{0.72}Nb_2O_6$ (*P*4*bm*, *a*=12.43Å, *c*=3.96Å). The experimental images were collected with a focus step of -26.6 Å on a JEOL-2100F transmission electron microscope equipped with field emission gun. The starting defocus of the series is determined to be -260 Å and the two-fold astigmatism is 33 Å with an azimuth angle of 13° clockwise with respect to the *x*-axis of the images. The reconstructed image is shown in the figure below, in which atoms appear as black dots. Not only metals but also atomic columns as light as oxygen can be seen.

The present method has the advantages of automatic defocus and two-fold astigmatism determination without amorphous areas, less CTF crossover problems and improved signal-to-noise ratio as compared to CTF correction methods using single images. The method has been implemented in a user-friendly program, *QFocus*, which we hope may help non-TEM experts to use HRTEM images for solving their structure problems.



[1] M. Haider, H. Rose, S. Uhlemann , E. Schwan, B. Kabius, K. Urban, *Nature* **1998,** *392*, 768-769. [2] W.M.J. Coene, A. Thust, M. Op de Beeck, D. Van Dyck, *Ultramicroscopy* **1996,** *64*, 109-135. [3] X.D. Zou, M. Sundberg, M. Larine, S. Hovmöller, *Ultramicroscopy* **1996,** *62*, 103-121.

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"Making the molecular movie": First frames…coming features

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One of the great dream experiments in Science is to watch atomic motions as they occur during structural changes. In the fields of physics, chemistry and biology, this prospect provides a direct observation of the very essence of chemistry and the central unifying concept of transition states in structural transitions. From a physics perspective, this capability would enable the observation of rarified states of matter at an atomic level of inspection, with similar important consequences for understanding nonequilibrium dynamics and collective phenomena. This experiment has been referred to as "making the molecular movie". Due to the extraordinary requirements for simultaneous spatial and temporal resolution, it was thought to be an impossible quest and discussed in the context of the purest form of a gedanken experiment. Recent developments in femtosecond electron guns with sufficient brightness to even execute single-shot structural determinations have made this experiment become a reality [1]. Previously thought intractable problems in attaining sufficient brightness and spatial resolution, with respect to the inherent electron-electron repulsion or space charge broadening, have been solved. With this new level of acuity in observing structural dynamics, there have been many surprises and this will be an underlying theme. Several movies depicting atomic motions during passage through structural transitions relevant to condensed phase dynamics will be shown [2], [3], [4]. The primitive origin of molecular cooperativity has also been discovered in recent studies of molecular crystals. These new developments will be discussed in the context of developing the necessary technology to directly observe the structure-function correlation in biomolecules –the fundamental molecular basis of biological systems. The future is even brighter with the advent of a new concept in relativistic electron guns that will open up direct observation of atomic motions in solution and