

The Atom TOMography (ATOM) Concept

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A major breakthrough in microscopy would occur if the unambiguous identities and true atomic coordinates of all the atoms in a volume could be determined. Neither of the current and distinct approaches to atomic scale microscopy, namely atom probe tomography (APT) and scanning transmission electron microscopy (STEM), can reach this ultimate goal at the present time. Therefore, a revolutionary Atom TOMography (ATOM) concept and project is being proposed that would create a new field of microscopy. In this atomic-scale tomography (AST) concept, the APT and STEM approaches are combined into a single instrument called the atomscope. This combination permits the full characterization of the structure and microstructure of the specimen to be determined at the atomic level. Not only could the local crystallography and solute distribution for all elements be evaluated in the atomscope, but the three-dimensional data could be used to generate many other types of information, such as the mechanical and electrical properties of the material.

The ultimate aims of the ATOM project are to integrate a local electrode atom probe (LEAP) into an aberration-corrected, ultrahigh vacuum scanning transmission electron microscope (STEM), and to develop a new type of single-atom position-sensitive detector with a detection efficiency of 100% for all the isotopes of the elements and with simultaneous measurement of the kinetic energy of the ions. The measurement of the kinetic energy of the ions will enable the overlap of ions with different mass-to-charge states to be resolved for fully quantitative compositional estimates. A new multi-axis stage and cryogenic sample holder that are capable of the sample movements required for electron tomography, including internal 360° rotation about the specimen axis, will be developed. The ability to perform 360° rotation will eliminate the missing wedge problem in electron tomography. The stage and sample holder will also incorporate a high voltage connection to the specimen and a single-use local electrode for APT. The atomscope will also incorporate an optical path to the specimen for laser-pulsed field evaporation. The incidence angle of the diffraction-limited focused laser beam will provide uniform illumination of the entire end form of the needle-shaped specimen to eliminate some local evaporation artifacts. The larger dynamic range, $\sim 10^6$, of available pulse-energies will enable a wide range of materials to be examined.

In addition to these hardware developments, both an evolutionary and revolutionary revision of the reconstruction algorithm of the atom positions and the data analysis software suite will be required to integrate the information from both electron microscopy/tomography and APT techniques. A fundamental limitation of TEM and APT is the lack of a feedback loop that may be used to verify the knowledge gained about a specimen. In the ideal case, a feedback loop exists where an image is obtained and a high quality model of the microscope's imaging process can then transform the image into the unique specimen that could have produced that image from that microscope. In practice, both TEM and APT are limited to feed-forward models, Fig. 1, i.e., an image of a specimen is obtained from the microscope and then a model of the microscope is used to calculate the image that is expected for the specimen. If the image predicted matches the image recorded, then it is hypothesized that the correct model for the specimen has been generated. However, it is

apparent from the information flow that the APT imaging process may be used as a feedback signal for the TEM imaging process. By combining the two techniques, an experimental solution to this long-time problem may be realized. A closed feedback loop may be achieved by combining TEM and APT images, as shown in Fig. 1. TEM tomography is the obvious image source for APT since it captures the entire specimen. Methods would also be developed to extract quantitative information from the resulting AST image.

The atomscope could be used in three main modes of operations in addition to stand alone conventional operation as a STEM and a LEAP. The first mode would be to perform electron tomography followed by atom probe tomography. Recently, APT and electron tomography data were obtained sequentially on the same sample in separate STEM and local electrode atom probe (LEAP[®]) instruments and then combined in a computer [1]. The second mode would be a time-sliced method to perform sequences of electron tomography, including high-resolution electron microscopy and/or surface profiling, followed by atom probe tomography. The third mode would be to do simultaneous electron tomography and atom probe tomography. [2]

- [1] I. Arslan, E. Marquis, M. Homer, M. Hekmaty, N. Bartelt, *Ultramicroscopy*, 108, 12 (2008) 1579-1585.
- [2] Research at the Oak Ridge National Laboratory SHaRE User Facility was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

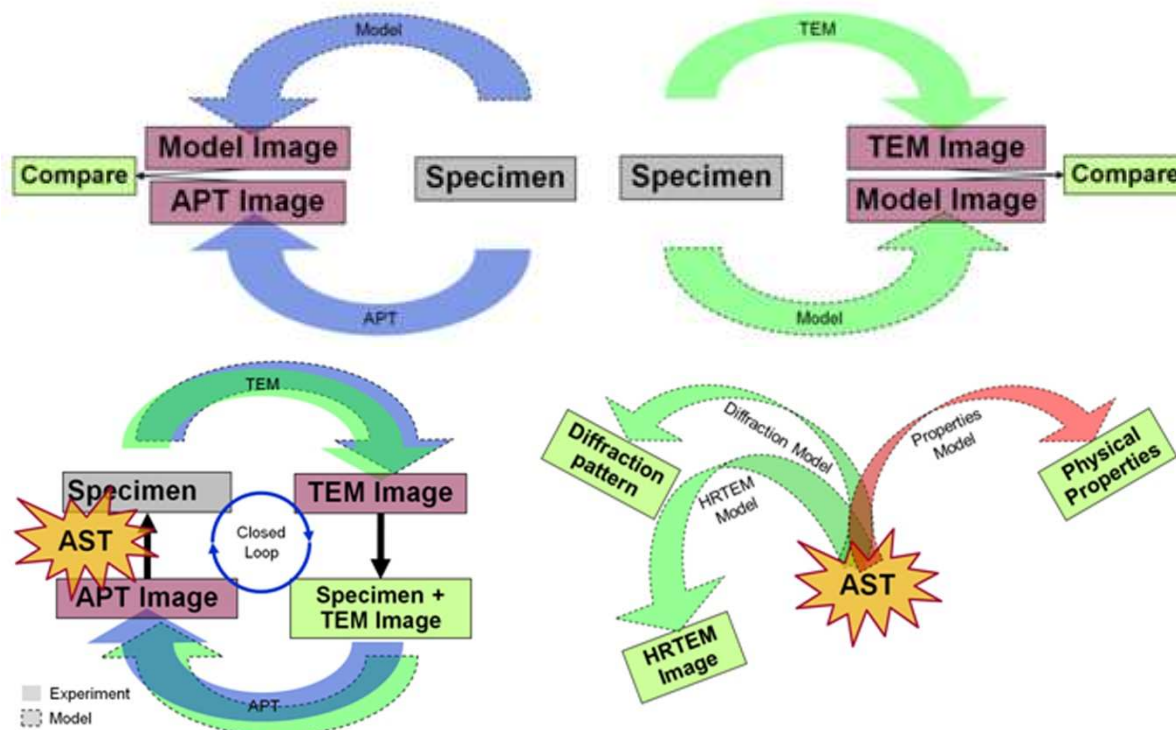


Figure 1 – The information loops for the APT, TEM, and the atomscope from the specimen to the final image. The atomscope loop is robust as it has both modeling and experimental components on each of the two key legs. Many types of information including images, diffraction patterns, and physical properties, etc., may be derived from the primary AST data.