OLIS: On-Line Image Simulation and structure characterization for the Materials Microcharacterization Collaboratory

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The Materials Microcharacterization Collaboratory (MMC)[1], a pilot project of the DOE2000 program, links DOE-sponsored electron microscope user facilities at ANL, LBNL, ORNL and UIUC with that at NIST to form one collaboratory. The MMC brings the microcharacterization and microanalysis tools available in these national centers to geographically-dispersed researchers working in industries, universities, and government laboratories. It enables remote users to share on-line the instrumentation, knowledge and expertise available at the individual facilities making up the collaboratory.

On-line services available to users of the MMC may be classified as instrument, computational, and exchange services (fig.1). LBNL's contribution to the MMC's instrumentation includes a Kratos EM-1500 HVEM (for remote in-situ high-voltage microscopy) and a Philips CM300 HREM (remote high-resolution capability). DeepView[2] is an exchange service that provides a common graphical user-interface (GUI) for control of MMC instruments over the wide area network (both the client and server sides of DeepView are available for download[3]). DeepView is cross-platform (able to work on a range of computers) and cross-microscope (able to control many kinds of TEMs and SEMs as well as their attached detectors such as EDS, GIF, PEELS, bi-prisms, and CCD cameras).

Computational services include on-line shape analysis and tracking for the Kratos and on-line software for the simulation of high-resolution electron microscope images and comparison with experiment by the remote user. Working from the early non-interactive HRTEM image simulation program SHRLI[4], O'Keefe[5] designed an NCEM upgrade called TEMPaS (for TEM Processing and Simulation) to provide NCEM users with an interactive menu-driven program for image simulation and comparison (the simulation module of TEMPaS is downloadable[6] under the name NCEMSS). A version of TEMPaS has now been modified for remote use and will be made available to remote users from an MMC URL under the name OLIS, for On-Line Image Simulation. Like the original TEMPaS, OLIS has an interactive GUI (fig.2) to allow users to enter and modify data interactively. OLIS can also be integrated with the DeepView GUI, and OLIS images can thus be displayed on the remote user monitor adjacent to the (live or captured) experimental image together with a difference image and a goodness-of-fit parameter (fig.3).

King[7] and Möbus[8] have shown that HRTEM image simulation can be used for structure refinement (QHREM) by iterative automatic modification of the model structure to achieve an optimum match of simulated and experimental images and thus refine the model structure. We plan to add such a structure-refinement module to OLIS to provide this feature to the on-line user. This module will use an MMC compute engine to run OLIS -- iteratively adjusting the model supplied by the user, computing the matching simulations, and displaying the current difference image and a plot of changes in the goodness-of-fit parameter. The final output would include notifying the user of the optimum best-fit model parameters.[10]

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9. M.A. O'Keefe, J.R. Taylor & D.K. Owen, in *56th Ann. Proc. MSA*, Atlanta, GA (1998) 42-43.
10. Work supported by Director, Office of Energy Research -- through the Office of Basic Energy Sciences, Material Sciences Division, and through the Office of Computational and Technology Research, Mathematical Information and Computational Sciences -- of the U.S. Department of Energy, under contract No. DE-AC03-76SF00098.

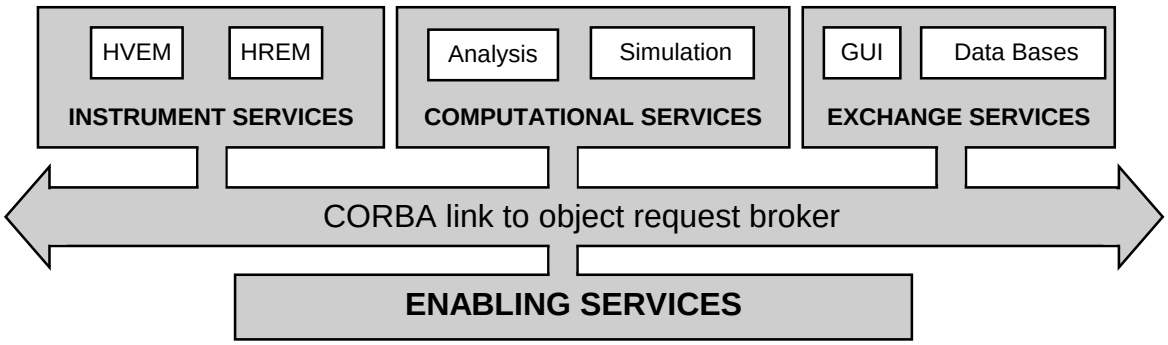

Figure 1: The three groups of on-line services provided by the MMC. Instrument services include access to microscopes such as the LBNL Kratos EM-1500 HVEM and Philips CM300UT/FEG HREM. Computational services include analysis tools to monitor shape changes of precipitates on the Kratos, as well as high-resolution on-line image simulation (OLIS) for users of the Philips.

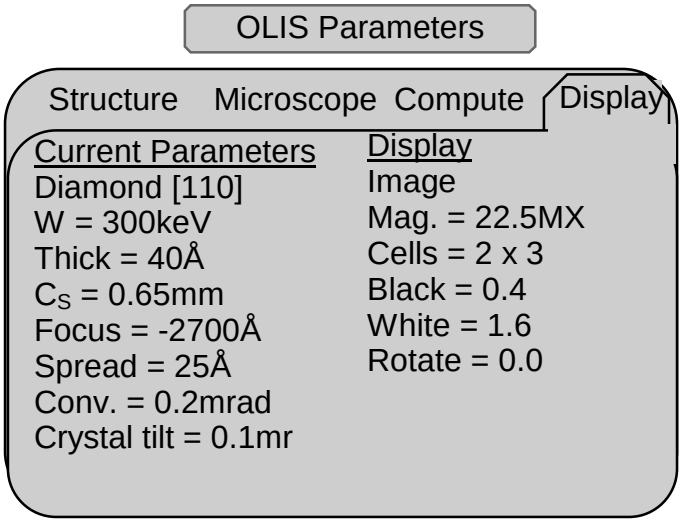

Figure 2: Prototype OLIS GUI provides for the input, subsequent adjustment, and display of structural, microscope, computational, and display parameters to the remote user.

Simulated diffraction patterns and images are displayed at the remote user terminal, either as tables computed for a range of conditions, or as single images. Single images can be computed and displayed in real time as the user changes parameter values. The user can choose to display accompanying contrast transfer functions (CTFs) and diffractograms.

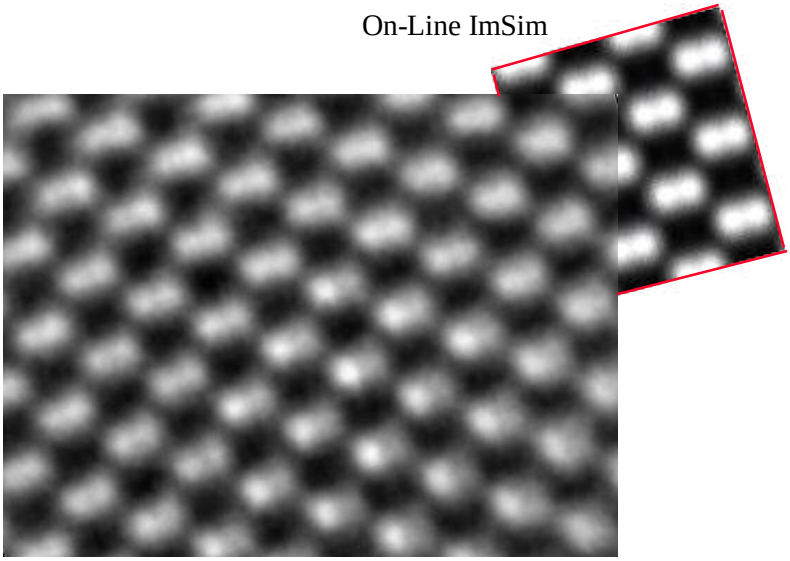

Figure 3: OLIS images can be superimposed on the DeepView (live) image at the remote user terminal. The figure shows an experimental image from the Philips CM300UT/FEG with an OLIS image that is computed for diamond in [110] orientation. As shown, the remote user can choose to "drag and drop" the simulated OLIS image onto the experimental DeepView image, and stretch and rotate it for better comparison with experiment.