1442
doi:10.1017/S1431927616008059
Microsc. Microanal. 22 (Suppl 3), 2016

Single-Slice Nanoworlds Online

P. Fraundorf[1-3], Stephen Wedekind[1], Taylor Savage[1], and David Osborn[2].

[1.] Physics & Astronomy Department, University of Missouri – St Louis, MO, 63121, USA
[2.] Center for NanoScience, University of Missouri – St Louis, MO, 63121, USA
[3.] Physics Department, Washington University – St Louis, MO, 63110, USA

Although general multi-slice calculations remain too slow, web-browsers on many platforms now make possible real-time single-slice (strong phase/amplitude object) simulation, with live image, diffraction, image power-spectrum, and darkfield-image modes, including specimen rotation e.g. for atomic-resolution images with specimens having several tens of thousands of atoms. Moreover, a wide range of qualitative phenomena emerge that include diffraction-contrast effects associated with thickness, orientation changes, and defect strain. Hence students with no math background can get a visceral feel for the way 2-D lattice-projections, diffraction-patterns, image power-spectra, aperture size/position, and darkfield images relate to a specimen's structure & orientation, as well as microscope contrast-transfer, well before access to a real electron microscope is available.

Artifacts from specimen-preparation aside, transmission electron-microscopy (TEM) involves the effective usage of electron-optics *plus* an understanding of beam-specimen interactions *as well as* insight into the structure of your particular specimen. Computer support for these characterization tasks is also evolving rapidly. However instrument-time for both operator-training and interface-development is limited and quite expensive.

Here we discuss the potential of strong phase/amplitude-object simulations, with help from JavaScript (JS) on modern (HyperText Markup Language or HTML version 5) devices, to serve up an online, mobile-friendly platform for TEM operator-training and analytical TEM software-interface development. The simulator that we make available has already been put to use with students in two NanoScience Practicals classes, and makes available real-time digital-darkfield tools useful with both deBroglie phase-contrast (e.g. high-resolution TEM) and incoherent amplitude-contrast (e.g. high-angle annular-darkfield scanning TEM or HAADF-STEM) lattice-images.

A surprising range of contrast-mechanisms (like thickness-fringes) manifest themselves (phenomenologically at least) without the need for slower multi-slice calculations. Microscopy-community ideas for new ``unknowns" to add, as well as new analytical-features for the software interface, are invited in this context.

Fig. 1 is screenshot of two live-captures, with phase-contrast brightfield at left and amplitude-contrast darkfield at right, of an “unknown” in our online simulator [1]. The electron-diffraction pattern in the top-right panel of each capture is found “upstream” in the electron wave-field as (to first order) the log-intensity power-spectrum of the specimen's projected-potential. Microscopists might think of it as a parallel-illumination selected-area diffraction-pattern of the region of the specimen in the field of view.

The centerpiece of the simulator (from which later panels are obtained) is the electron-optical image in the top-left panel, which is recorded “downstream” of the microscope's imaging lenses. It is affected by the microscope's damping-envelope and spherical-aberration coefficient (presently fixed), as well as by lens focus-settings [2] which are adjustable with buttons above the top row of panels.

When the page is loaded, the focus setting of the system is randomized (in the same way for all “unknowns”), so that a (one-time) exercise in correcting astigmatism and optimizing focus may be needed. All panels of course are affected by specimen orientation, which along with unknown choice and darkfield aperture size are selected with buttons below the top row of panels.

The panel at bottom-right is a (log-intensity) power-spectrum of the electron-optical image at top-left. In this panel the spherical-aberration zeros in the contrast-transfer function are useful for focus and astigmatism correction, as well as for understanding lens effects on the images. The panel also contains the moveable digital-darkfield aperture, which behaves like a physical aperture in the diffraction pattern. The resulting digital-darkfield image [3] is shown in logarithmic complex-color in the bottom-left panel.

References:

[1] under Nanostructure Explorer @ https://sites.google.com/site/electrondetectives
[2] E. J. Kirkland, Advanced Computing in Electron Microscopy 2nd ed. (2010) Plenum Press NY.
[3] P. Fraundorf, M&M 20 (2014) 824-825 and earlier.

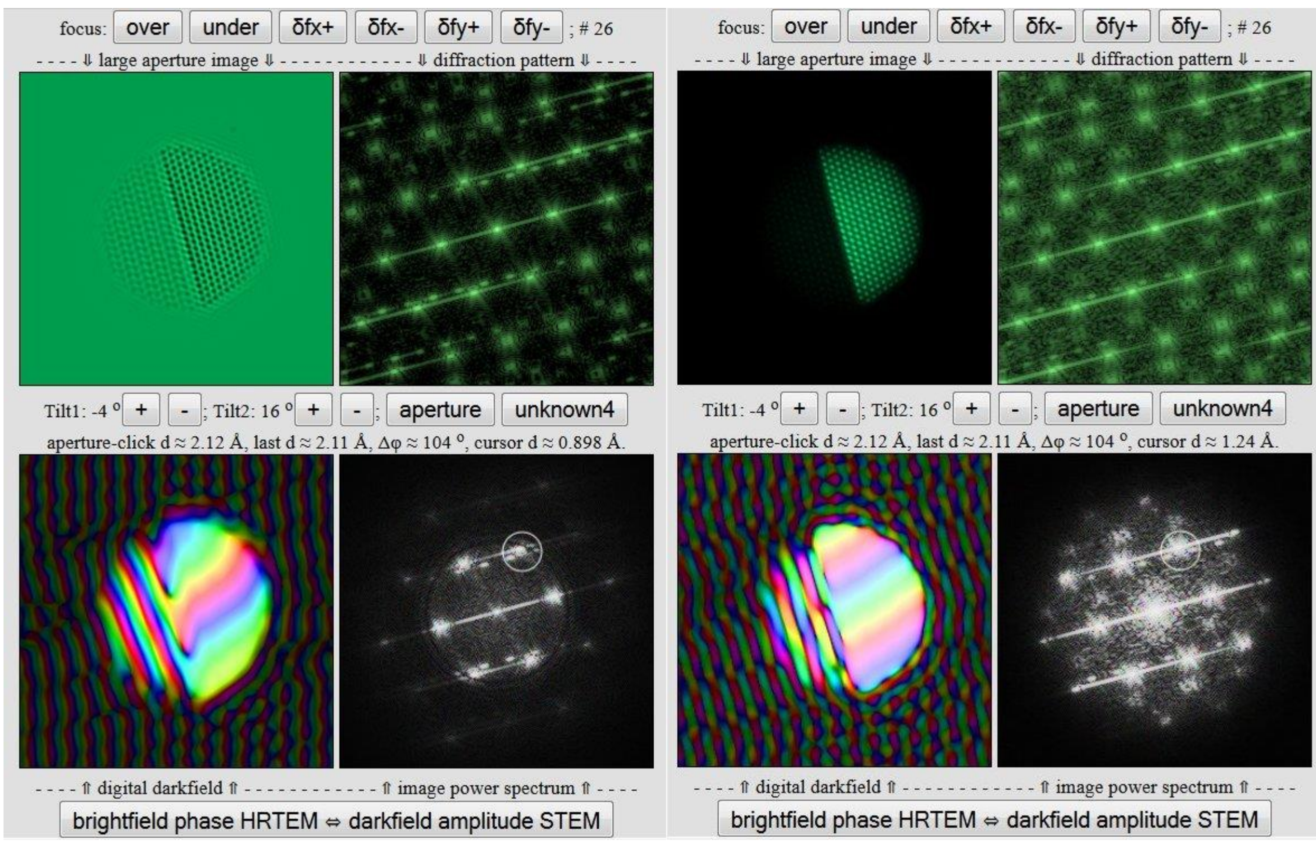

Figure 1. Brightfield high-resolution TEM (phase) and darkfield scanning-TEM (amplitude) screenshots of an ``unknown" specimen in an online simulator, with the same defocus, orientation, and darkfield-aperture.

https://doi.org/10.1017/S1431927616008059 Published online by Cambridge University Press