

# Complex-Color Darkfield TEM Interfaces for Crystal, Defect, & Strain Analysis

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**Introduction:** Imaging of a specimen using one or more beams diffracted by that specimen, i.e. optical darkfield imaging, is a powerful tool in electron microscopy, with applications ranging from high angle annular darkfield imaging of single atoms to weak beam imaging of strain around nuclear particle tracks in crystals. A very similar technique can be used on digitized electron images of specimens, with the added bonus that Fourier phase information (not available in optical darkfield images) can be incorporated directly into the images using “complex color”. This information can provide quantitative data on picometer-scale spacing variations, and vector strain, in periodic structures [1]. In off-line analysis, the latter has been referred to as strain mapping, but computer support for microscopes today can make this viscerally available to microscope operators in real time. In this paper, we discuss (i) on-line implementation of this digital darkfield functionality, (ii) how to interpret the color images, and (iii) web based simulators which allow you to get a feel for its use in a variety of applications.

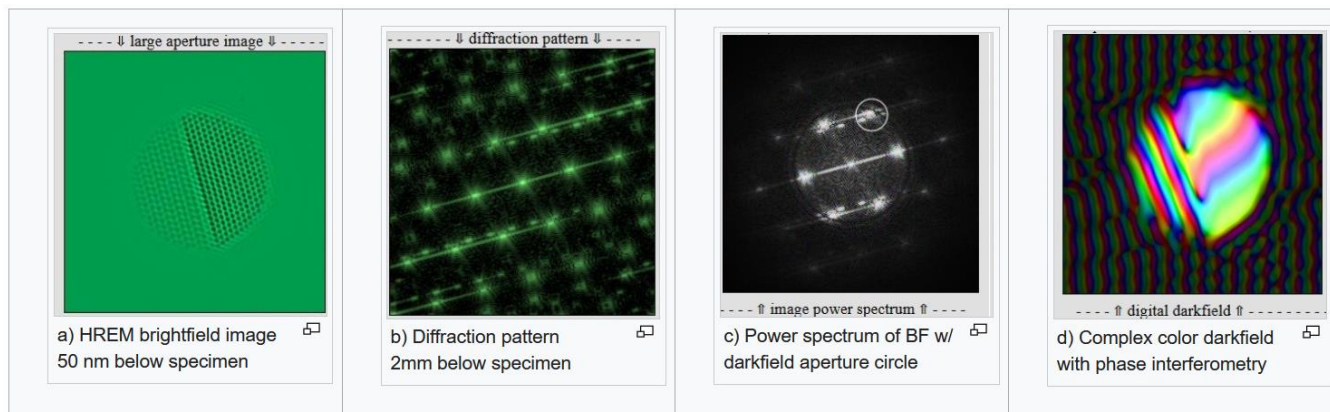
**Methods - Mathematics, Visualization, Algorithms:** Optical darkfield imaging is an analog form of wavelet-like decomposition, intermediate between direct and reciprocal space [2]. Needless to say, therefore, it can also be done digitally, with the added benefit that phases as well as squared-amplitudes (intensities) can be recovered in the process. Since the resulting 2D field is a field of complex numbers, we visualize these fields (e.g. as in a recent sound visualization patent [3]) using the cyclic color field called "hue" (from red = 1 to chartreuse = i to cyan = -1 to indigo = -i) for denoting the phase angle in polar form. Intensity and amplitude as usual are denoted with brightness (below 1) and saturation (above 1). Real time single-slice (strong phase-object) optical modeling [4,5] can be done in real-time using fast Fourier transform algorithms, with small images even in a browser on-line [6].

**Color Image Interpretation:** Interpretation of these complex color images takes a little practice. It is the changes in color across the field of view, rather than the absolute color itself, that is usually of interest. For instance, if the darkfield aperture is centered on a diffraction spot from an unstrained uniformly-thick crystal lattice, that region of the image where that lattice is located will be uniform in color. Regions in the same image where the lattice spacing is only slightly different will show stripes perpendicular to the offset of the region's diffraction spot from aperture center cf. Fig 1. Moving the aperture off center of the diffraction spot will, similarly, create stripes perpendicular to the offset, which (like the beats when tuning two musical instruments) get closer together as the offset increases. Places in the image with no periodicities, and/or with periodicities that fall outside the diffraction aperture, remain dark. This interferometry, like that used by LIGO for gravitational astronomy, can be exquisitely sensitive e.g. in this case to periodicity-differences orders of magnitude below the microscope's resolution.

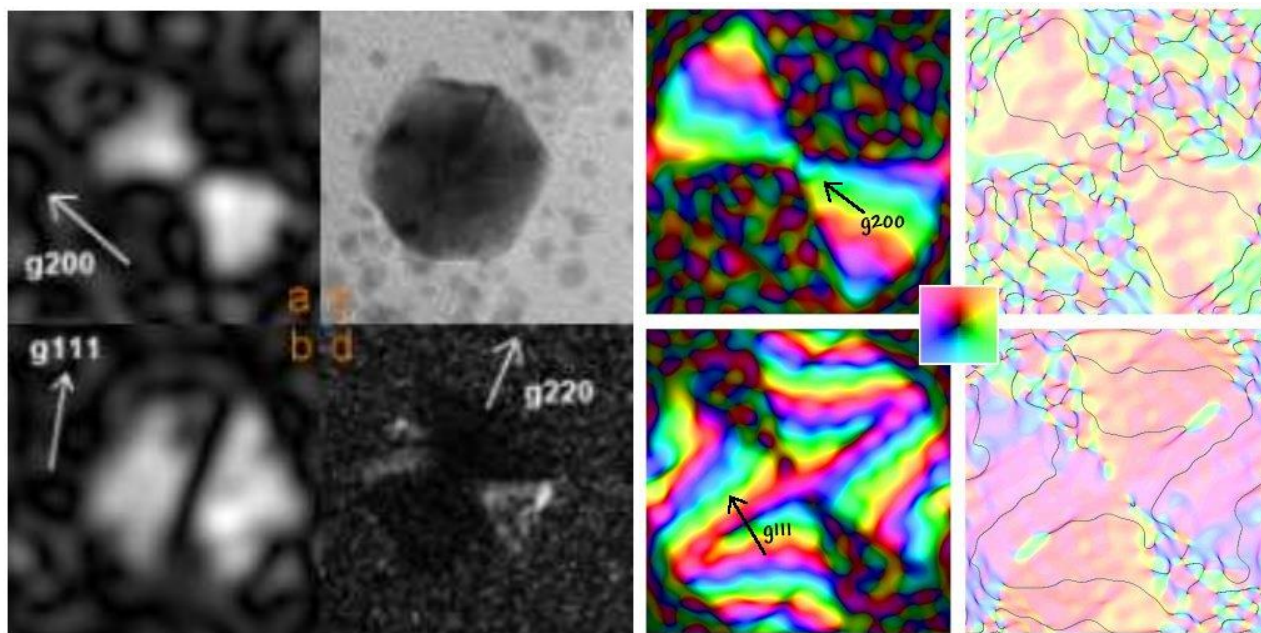
**Applications:** Like optical darkfield, digital darkfield can be used to see what objects in an image are giving rise to any particular diffraction spot. In a field with multiple crystals, it can be used to obtain diffraction information on individual crystals cf. Figs. 2 & 3. In fact, if data is taken before and after tilting, one can even use the diffraction spot spacings and angles to determine the unique 3D oriented basis triplet (and lattice parameters) for a given crystal. By choosing specific diffraction spots from a single crystal, it can similarly be used to determine the Burger's vector of dislocations, and to determine the crystal planes involved in strain around inclusions (e.g. to see if the interface is coherent or not). Using the Fourier phase information, it further allows one to quantify projected strain magnitude and direction, e.g. around lattice

defects and at the interface between layers e.g. in Si/Ge semiconductors. Very slight differences in lattice parameters, e.g. associated with quantum dots in a structure, can be visualized as well.

On-line Simulation, and Practice: To offer a feel for how this would work in the interface to your microscope(s), and to show that digital darkfield imaging can be made available on digital images in real time, this functionality has been incorporated into our on-line JS/HTML5 strong phase object simulator [7]. If there are specific specimen types that you would like to see made available in that simulator, let us know.



**Fig. 1.** Simulated ZnO/Au bi-crystal sphere 11.2nm field-width image series: brightfield, diffraction, image power spectrum with darkfield aperture, resulting digital darkfield image in complex color.



**Fig. 2.** Sub-crystal digital darkfields of randomly oriented Pd icosahedral twin w/2nm fieldwidth BF; **Fig. 3.** Simulated color digital darkfield images of subcrystals in a 10 “bowtie” crystal icosahedral twin.

References:

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