Interpretation of electron holographic phase images and defocused bright-field images of nanocarbon field emitters

F Ubaldi[1], T Kasama[2], G Pozzi[1] and R E Dunin-Borkowski[2]

1. Department of Physics, University of Bologna, 40127 Bologna, Italy
2. Center for Electron Nanoscopy, Technical Univ. of Denmark, Lyngby, Denmark

filippo_ubaldi@yahoo.it
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Electron holography is well suited to the investigation of electric and magnetic fields at the mesoscopic scale, in part because equiphase lines generated from reconstructed phase images can provide a visually compelling image of the distribution of the projected electrostatic potential or magnetic induction. Although it is tempting to interpret such phase contours directly in terms of the electrostatic potential or the magnetic lines of force within and around a specimen, three-dimensional modeling is in general required to understand the three-dimensional field distribution accurately [1].

The need to compare an experimental phase image with simulations is demonstrated by Fig. 1a, which shows equiphase lines recorded using off-axis electron holography from a wire comprising a bundle of single-walled carbon nanotubes that have a voltage applied to them *in situ* in the electron microscope. Figure 1b shows a corresponding out-of-focus image recorded from a similar wire [2]. These images cannot be interpreted using a previous model based on the electrostatic potential of a line charge of constant density [3]. A more realistic analytical model can be constructed starting from a line with a linearly increasing charge density, modeled as a rotation ellipsoid immersed in a constant electric field (with the charge density decreasing to zero at its mid-point) [4, 5]. In this case, the integrated potential can be obtained analytically, and the resulting equiphase lines (Fig. 2a) show better agreement with the experimental result. However, the agreeement with the recorded out-of-focus image is still poor, especially at the tip of the nanotube bundle (Figs. 2b and 1b).

A better fit to the experimental results is obtained by using ab-initio numerical modeling based on the commercial software tools ISE-tCad tools Mesh and DESSIS. The results of such a calculation are shown for a cylindrical nanotube in Figs. 3a and 3b, which show numerical simulations of equiphase lines and an out-of-focus image, respectively. The qualitative agreement with the experimental results is now improved, presumably because the numerical calculation provides a better model for the true shape of the wire and in particular for the charge distribution along its length, which is now non-linear [6].

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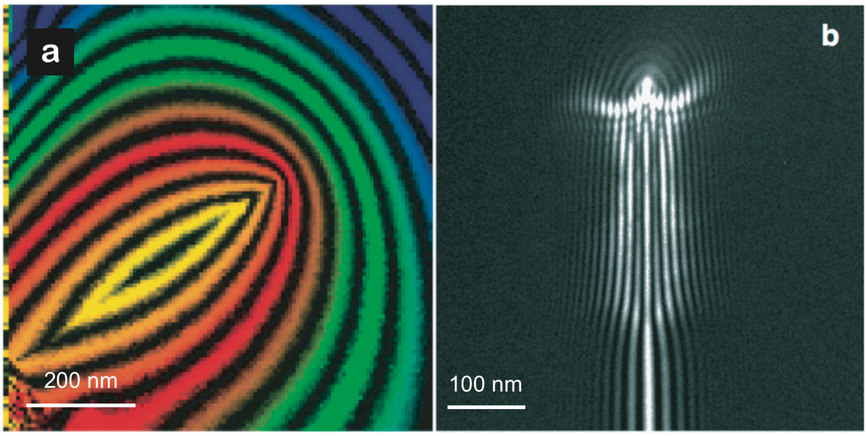

Figure 1. a) Contoured phase image obtained from an off-axis electron hologram and b) a defocused bright-field image of the end of a bundle of single-walled carbon nanotubes that has a voltage applied to it *in situ* in the TEM.

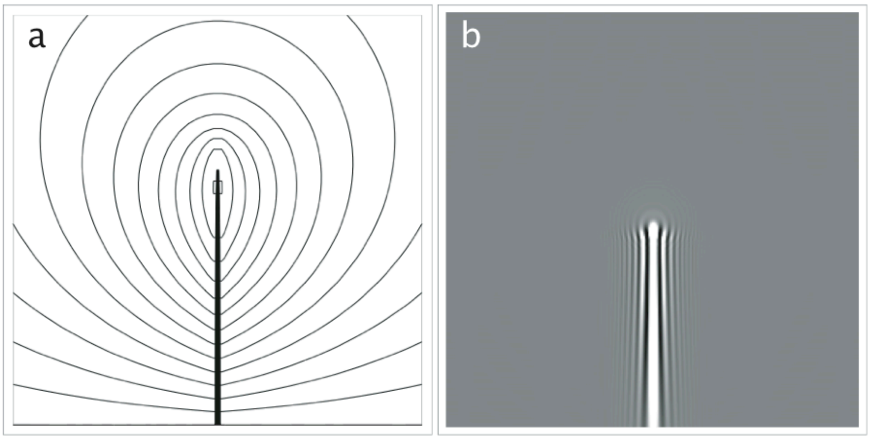

Figure 2. Analytical simulations of an ellipsoidal nanotube (black) of a) phase contours and b) an out-of-focus image.

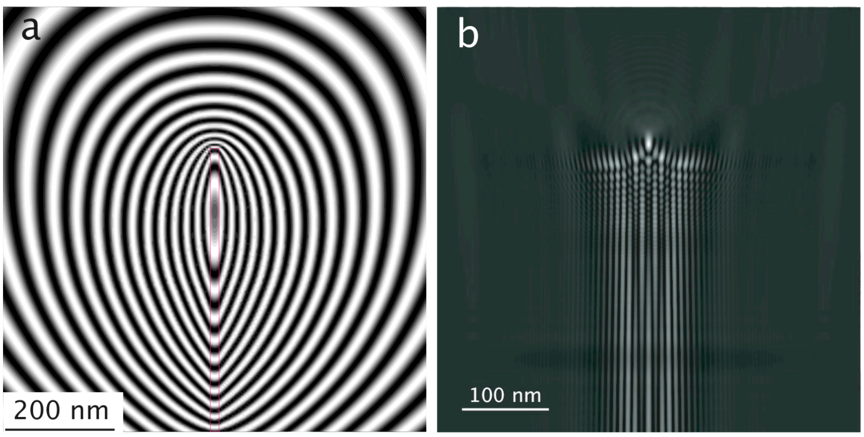

Figure 3. Numerical simulations of a) phase contours and b) an out-of-focus image of a cylindrical nanotube, obtained by integration of the electrostatic potential computed using the commercial software ISE-tCad.

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