# Model-based iterative reconstruction of charge density and electric field using off-axis electron holography

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The ability to measure local variations in charge density in the transmission electron microscope would provide a valuable tool for the study of functional materials ranging from ferroelectrics to semiconductors. Similarly, the ability to measure local variations in electric field outside electrically-biased needle-shaped samples would be of great importance for understanding the fidelity and spatial resolution of reconstructions of microstructure and chemical composistion achieved using atom probe tomography [1, 2], in particular for samples that contain multiple phases or insulating materials. Off-axis electron holography is a powerful technique that provides direct access to the phase of the high energy electron wave that has passed through a sample in the transmission electron microscope [3]. In the absence of magnetic fields, the phase is sensitive to the electrostatic potential in the specimen projected in the electron beam direction. The local projected charge density in the specimen can in principle be determined directly from the Laplacian of a recorded phase image. However, such a model-independent approach suffers from poor signal-to-noise, as well as from artefacts associated with local variations in mean inner potential and specimen thickness [4]. Here, we describe a model-based iterative technique that can be used to reconstruct the projected charge density distribution inside a specimen from a single electron optical phase image measured using off-axis electron holography, or alternatively the three-dimensional charge density distribution from a tomographic tilt series of phase images [5]. We use a forward model in an iterative algorithm to solve the inverse problem of reconstructing the charge density in the specimen, as shown in Fig. 1. Additional constraints and known physical laws can be incorporated in the solution. For the three-dimensional problem, such a model-based approach avoids many of the artifacts that result from the use of classical tomographic techniques. If required, the projected or three-dimensional electric field can then be determined numerically from the reconstructed charge density. Figure 2 illustrates the reconstruction of the projected charge density distribution in an atom probe tomography needle, which contains a conducting base and an insulating $Al_2O_3$ apex. Here, the needle is unbiased, but becomes charged in the absence of an applied voltage as a result of exposure to electron beam irradiation. Off-axis electron holograms of the needle were recorded at 300 kV using a Gatan K2 camera in an FEI Titan TEM equipped with an electrostatic biprism. Experimental equiphase contours are shown in Fig. 2(a). Corresponding simulated equiphase contours, which were generated from the best-fitting reconstructed charge density distribution in the specimen, are shown in Fig. 2(b) and are consistent with the experimental phase image in the vacuum region outside the specimen. The challenges of developing this algorithm, as well the uniqueness of the solution and its sensitivity to boundary conditions, will be discussed [6].

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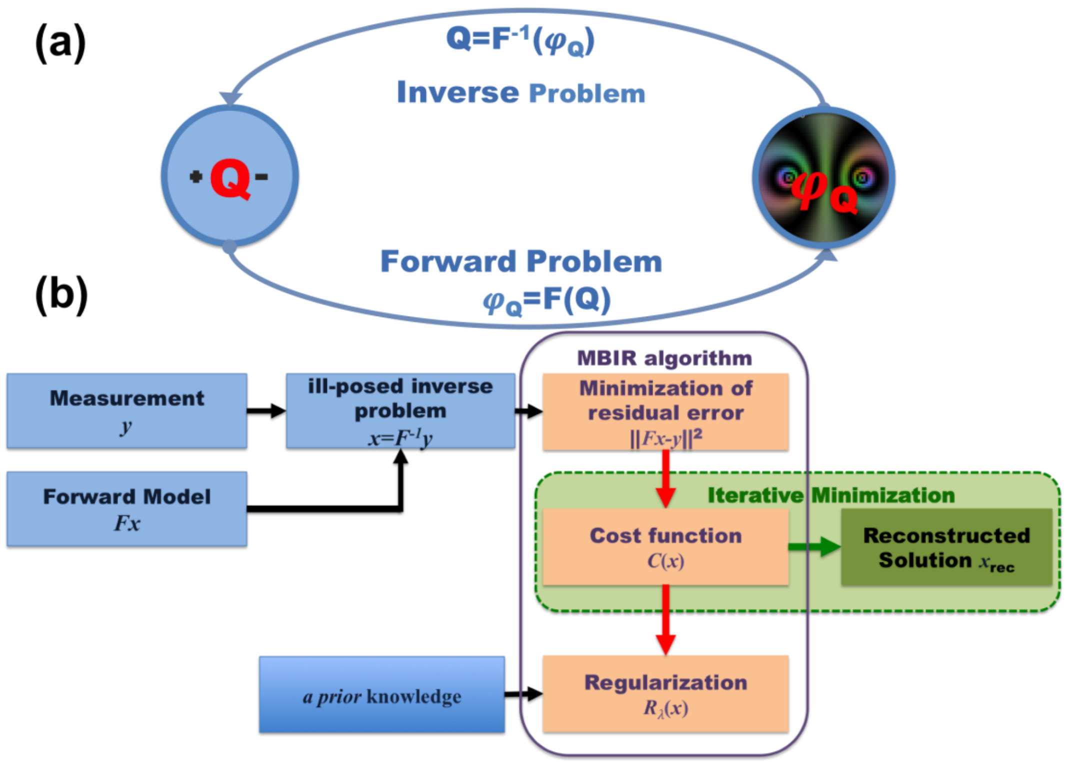


**Fig. 1** (a) Schematic diagram illustrating the forward and inverse problems that link the charge distribution Q with the phase shift $\varphi_Q$. (b) Workflow of the reconstruction process used here to solve the ill-posed inverse problem.

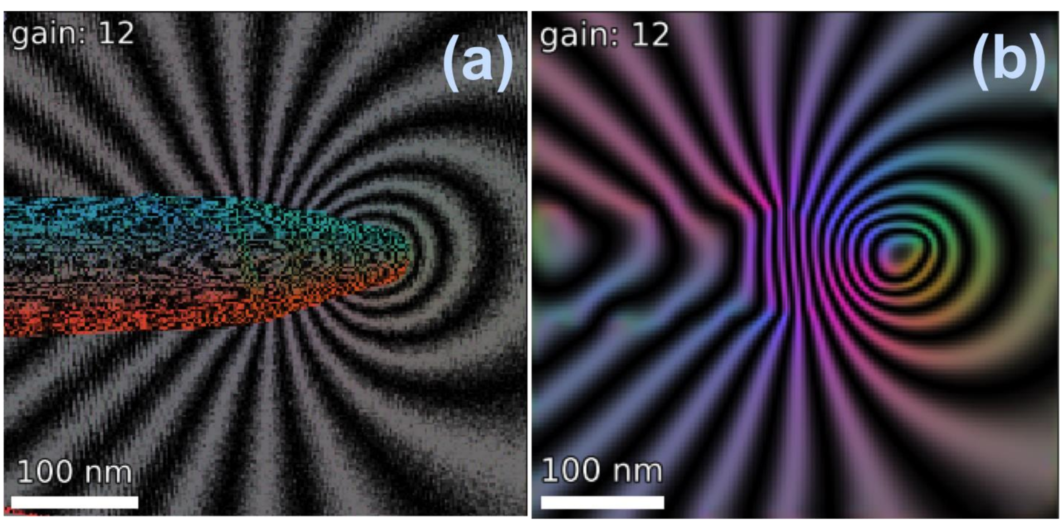


**Fig. 2** Example of the reconstruction of tge charge density distribution in an atom probe tomography needle that has an insulating $Al_2O_3$ apex. (a) Experimental phase contour map. The phase contours inside the needle are affected by the mean inner potential of the specimen. (b) Simulated phase contour map determined from the best-fitting charge density distribution in the specimen, which was reconstructed only from the phase shift measured in vacuum outside the needle. The phase contour spacing is $\pi/6$ radians.