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3D reconstruction of the magnetic vector potential using model based iterative reconstruction

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A B S T R A C T

Lorentz transmission electron microscopy (TEM) observations of magnetic nanoparticles contain information on the magnetic and electrostatic potentials. Vector field electron tomography (VFET) can be used to reconstruct electromagnetic potentials of the nanoparticles from their corresponding LTEM images. The VFET approach is based on the conventional filtered back projection approach to tomographic reconstructions and the availability of an incomplete set of measurements due to experimental limitations means that the reconstructed vector fields exhibit significant artifacts. In this paper, we outline a model-based iterative reconstruction (MBIR) algorithm to reconstruct the magnetic vector potential of magnetic nanoparticles. We combine a forward model for image formation in TEM experiments with a prior model to formulate the tomographic problem as a maximum a-posteriori probability estimation problem (MAP). The MAP cost function is minimized iteratively to determine the vector potential. A comparative reconstruction study of simulated as well as experimental data sets show that the MBIR approach yields quantifiably better reconstructions than the VFET approach.

1. Introduction

In a Lorentz transmission electron microscopy (LTEM) experiment, an electron propagating through a thin specimen experiences a Lorentz Force $\mathbf{F}_L = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ [1] due to the sample's electrostatic field, $\mathbf{E}$, and magnetic field, $\mathbf{B}$; $-e$ is the electron's charge and $\mathbf{v}$ its velocity. This (classical) force generates a deflection of the electron trajectory, which can be used to explain the Fresnel and Foucault observation modes [2]. A more robust explanation of the nature of the electron-specimen interaction involves quantum mechanics, in which the electron is described by a wave function $\psi(\mathbf{r}_\perp) = a(\mathbf{r}_\perp)e^{i\varphi(\mathbf{r}_\perp)}$ [2]. Elastic scattering in the sample produces variations of the amplitude $a(\mathbf{r}_\perp)$, whereas the electromagnetic potentials affect the phase $\varphi(\mathbf{r}_\perp)$ of the wave; $\mathbf{r}_\perp$ is a vector normal to the propagation direction. Aharonov and Bohm [3] showed, in 1959, that the phase of the exit wave function encodes information on the sample' s electrostatic potential, $V(\mathbf{r}_\perp, z)$, and magnetic vector potential, $\mathbf{A}(\mathbf{r}_\perp, z)$, as follows:

$$\varphi(\mathbf{r}_\perp) = \varphi_e(\mathbf{r}_\perp) + \varphi_m(\mathbf{r}_\perp) = \frac{\pi}{\lambda E_t}\int_L V(\mathbf{r}_\perp, z)dz - \frac{e}{\hbar}\int_L \mathbf{A}(\mathbf{r}_\perp, z)\cdot d\mathbf{r}, \quad (1)$$

where $\hbar$ is the reduced Planck's constant, E_t is the total beam energy, and the integrals are carried out along the beam direction, L. The total phase shift, φ, consists of an electrostatic contribution, φ_e, and a magnetic contribution, φ_m. The phases are not directly observable, but their effect on the image contrast can be determined by considering the point spread function, $\mathcal{T}_L(\mathbf{r}_\perp)$, of the Lorentz lens. The image intensity is then given by the modulus-squared of the convolution product $\psi(\mathbf{r}_\perp) \otimes \mathcal{T}_L(\mathbf{r}_\perp)$ [2]. Hence, characterization of the electromagnetic potentials begins with phase shift retrieval from the image intensities, using either electron holography [4] or the transport-of-intensity equation (TIE) formalism [5], which is based on a through-focus series of Fresnel images. We use the linearity of the TIE [6] and time reversal symmetry to retrieve the individual phases φ_e and φ_m.

Characterization of the electromagnetic fields is then achieved by performing scalar field and vector field tomographic recon-

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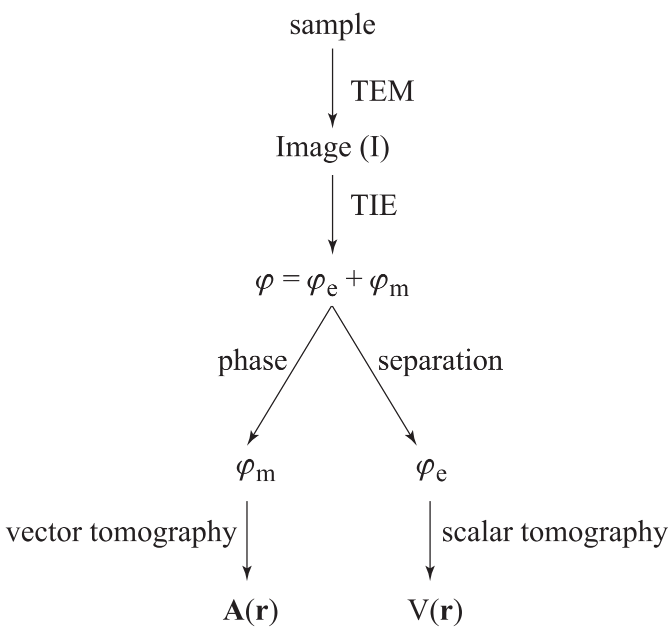

Fig. 1. A flow chart illustrating the methodology to determine electromagnetic potentials of a magnetic nanoparticle sample.

structions to determine $V(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$, respectively. We refer to the use of vector field tomography to reconstruct the electromagnetic potentials as Vector Field Electron Tomography (VFET) [7]. A schematic of the operations performed to complete an electromagnetic characterization task is shown in Fig. 1.

In this contribution, we primarily focus on vector field tomography to reconstruct $\mathbf{A}(\mathbf{r})$. In recent years, the VFET approach employed the filtered back projection (FBP) approach to perform the reconstructions [8,9]. Although FBP yields a good estimate with a complete set of measurements, the typical missing wedge of TEM data significantly diminishes the quality of the reconstructions [10]. In addition, typical tilt series are obtained using an angular step size of 2°–5° to minimize the necessary pre-processing steps (image alignments) and reduce beam damage. These limitations, collectively, yield a reconstruction result that can exhibit substantial artifacts. To alleviate these problems, we resort to a more robust and statistically based tomographic reconstruction framework known as model-based iterative reconstruction (MBIR) to determine $\mathbf{A}(\mathbf{r})$. This approach has had considerable success in improving reconstruction quality in scalar tomography [11,12].

In Section 2, we briefly outline conventional VFET and show how we can reconstruct all three component of $\mathbf{A}(\mathbf{r})$ from just two tilt series; we also perform an error analysis of the quality of VFET reconstructions in the presence of a missing wedge. Next, in Section 3, we provide an overview of the MBIR framework, and in Section 4, we incorporate MBIR into the reconstruction of $\mathbf{A}(\mathbf{r})$ and compare the results with those from conventional VFET reconstructions.

2. Vector field electron tomography

Vector field tomography is relatively new; it was not until 1988 when Norton [13], for the first time, outlined a mathematical model to determine the 2D fluid field from acoustic time travel measurements. Subsequent years saw extensions of 2D vector tomography to 3D cases; in particular, Juhlin [14] resolved the solenoidal part of a divergence free flow field using ultrasound Doppler measurements in 1992. In 2005, Lade et al. [8] presented the VFET model to reconstruct 3D vector fields from longitudinal and transverse measurements. In 2008, Phatak et al. [15] used the

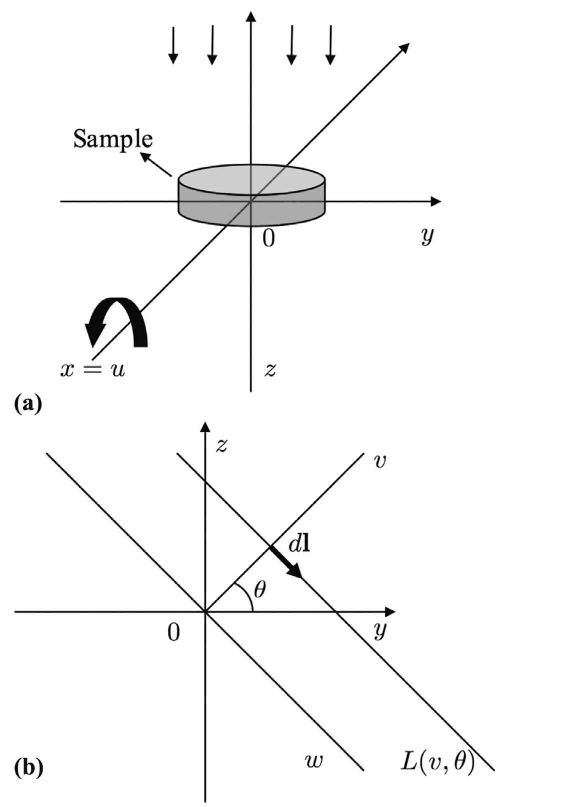

Fig. 2. (a) Illustration of phase shift acquisition for an x-tilt series with the arrows representing the electron propagation direction and the curved arrow indicating counter-clockwise sample rotation. (b) Representation of the reference frame used to express the differential vector element $d\mathbf{l}$.

VFET approach to reconstruct the magnetic vector potential and induction of magnetic nanoparticles. Since this VFET model is still relevant for our new MBIR method, we devote this section to a brief review of the VFET framework.

Since tomographic reconstructions require a forward model to project the object being reconstructed, we begin by considering the computation of the magnetic phase shift. The relation $\varphi_m(\mathbf{r}_\perp) = -\frac{e}{\hbar}\int_L \mathbf{A}(\mathbf{r}_\perp, z) \cdot d\mathbf{r}$ describes the magnetic phase shift obtained at 0° tilt. To obtain the phase shift for a tilted sample we consider a tilt series around the x axis (counterclockwise); the new coordinate vectors, $\mathbf{t}$, can be expressed in terms of the original ones, $\mathbf{r}$, by $\mathbf{r} = R_{\theta,x}\mathbf{t}$ where $\mathbf{r} = [x\ y\ z]$, $\mathbf{t} = [u\ v\ w]$, and $R_{\theta,\,x}$ is the counter-clockwise rotation matrix (Fig. 2(a)). From Fig. 2(b), the vectorial line element, $d\mathbf{l}$, of the projection line $L(v, \theta)$, can be written as $d\mathbf{l} = [\hat{y}\sin(\theta) - \hat{z}\cos(\theta)]dl$.

Writing $\mathbf{A}(\mathbf{r}) = A_x(x, y, z)\hat{x} + A_y(x, y, z)\hat{y} + A_z(x, y, z)\hat{z}$, a generic projection equation for the x tilt series in Fourier space, $\tilde{\varphi}_{m,x}$, can be obtained as:

$$\tilde{\varphi}_{m,x}(k_u, k_v) = -\sin\theta \tilde{A}_y(k_u, k_v\cos\theta, k_v\sin\theta) + \cos\theta \tilde{A}_z(k_u, k_v\cos\theta, k_v\sin\theta); \tag{2}$$

a similar analysis for the y tilt series produces

$$\tilde{\varphi}_{m,y}(k_u, k_v) = -\sin\theta \tilde{A}_x(k_u\cos\theta, k_v, k_u\sin\theta) + \cos\theta \tilde{A}_z(k_u\cos\theta, k_v, k_u\sin\theta). \tag{3}$$

Eqs. (2) and (3) represent the Fourier slice theorem for 3D vector fields for x tilt series and y tilt series respectively.

The formulation of the reconstruction procedure by means of the VFET approach begins by imposing a gauge constraint on the magnetic vector potential, i.e., $\nabla \cdot \mathbf{A} = 0$. This constraint is written