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Comparing Fourier optics and contrast transfer function modeling of image formation in low energy electron microscopy

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ABSTRACT

A theoretical understanding of image formation in cathode lens microscopy can facilitate image interpretation. We compare Fourier Optics (FO) and Contrast Transfer Function (CTF) approaches that were recently adapted from other realms of microscopy to model image formation in low energy electron microscopy (LEEM). Although these two approaches incorporate imaging errors from several sources similarly, they differ in the way that the image intensity is calculated. The simplification that is used in the CTF calculation advantageously leads to its computational efficiency. However, we find that lens aberrations, and spatial and temporal coherence may affect the validity of the CTF approach to model LEEM image formation under certain conditions. In particular, these effects depend strongly on the nature of the object being imaged and also become more pronounced with increasing defocus. While the use of the CTF approach appears to be justified for objects that are routinely imaged with LEEM, comparison of theory to experimental observations of a focal image series for rippled, suspended graphene reveals one example where FO works, but CTF does not. This work alerts us to potential pitfalls and guides the effective use of FO and CTF approaches. It also lays the foundation for quantitative image evaluation using these methods.

1. Introduction

Progress in understanding the properties of advanced materials is made possible by the availability of a broad range of experimental characterization techniques. Low energy electron microscopy (LEEM), spin polarized LEEM (SPLEEM) and photoemission electron microscopy (PEEM) are forms of cathode lens microscopy that have grown into preeminent *in-situ* imaging techniques for the study of the morphological, structural, chemical, electronic and magnetic properties of surfaces, ultra-thin films and surface-supported nanostructures [1–6]. With the improved resolution that has been achieved due to the advent of aberration-corrected instruments based on mirror correctors in recent years, even greater progress using LEEM, SPLEEM and PEEM can be expected in the future [7–11]. However, capitalizing on the capabilities of these techniques also depends upon advances in our theoretical understanding of image formation and contrast.

An early effort to understand image formation in LEEM was targeted narrowly at modeling phase contrast that occurs at atomics steps. At an elementary level, step contrast arises due to the interference of electron waves that are reflected from terraces on the opposite sides of a step. A wave-optical model of step contrast was developed [12] as an extension to a suitable optical analog that was reported much earlier [13]. This model provided a deeper qualitative understanding of step contrast. However, a key shortcoming of this approach is that it essentially treats the case of an ideal instrument with aberration-free imaging and a perfectly coherent electron source. Imaging errors that come from a variety of sources in real instruments could only be included conceptually in an *ad hoc* way.

Telieps first suggested thirty years ago that image formation in LEEM could be addressed using more sophisticated methods that incorporate the effect of the imaging system rigorously [14]. This idea was eventually realized when Fourier Optics (FO) and Contrast Transfer Function (CTF) approaches were adapted from other realms of microscopy [15–17], notably optical microscopy and transmission electron microscopy (TEM), to model image formation in conventional (uncorrected) and aberration-corrected cathode lens microscopy [18–23]. These two related modeling approaches incorporate imaging errors that are introduced by several sources, including lens aberrations, defocus, spatial and temporal coherence and diffraction. A recent application of FO facilitated the practical interpretation of contrast that was observed for a strained MnAs film on a GaAs substrate [23]. The self-organization of the film into a periodic stripe array with ridge-groove morphology pro-

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duces an unusual 'duplex' phase contrast under defocus conditions. The intrinsic widths and the ridge height were determined quantitatively by comparison of experimental observations of contrast in a focal image series to FO model simulations. This work demonstrates how CTF and FO methods may be used to carry out quantitative image evaluation. It also highlights the importance of energy-dependent and focal image series for this purpose.

Although FO and CTF modeling approaches incorporate imaging errors in the imaging wave in the same way, they differ critically in how the image intensity is calculated from the modified imaging wave. The FO method is mathematically rigorous and should be generally valid. On the other hand, a simplification of the intensity calculation in the CTF approach incorrectly treats some of the effects arising from the limited spatial and temporal coherence of the illumination. This simplification advantageously leads to the computational efficiency of the CTF method. However, the validity of the CTF method for modeling the strong phase and amplitude objects that are frequently encountered in cathode lens microscopy remains unclear. In this paper, factors that may affect the validity of the CTF approach for modeling image formation in LEEM are identified. This is done by examining how the mathematical formalism of the CTF and FO approaches differ and by comparison of CTF and FO image simulations for several test objects and experimental results. This allows an understanding of the conditions that the CTF approach is valid and when the rigorous FO method must be used.

2. Image formation theory

2.1. Imaging principle

In cathode lens microscopy, images are formed using electrons that are emitted from the sample [1–6]. Electron emission may be stimulated by external illumination via elastic or inelastic processes. In LEEM, electrons are emitted by elastic back-scattering of a collimated low energy electron beam. Emitted electrons are accelerated from their typically low emission energy, E_0, to considerably higher kinetic energy, E, in the strong and nearly uniform electric field between the sample (cathode) and the first electrode (anode) of the cathode objective lens. The deflection of electron trajectories that occurs during acceleration in a uniform field produces a virtual object behind the sample with unity magnification [24–26]. A small opening is present in the first electrode that allows electrons to pass through the electrode. This opening acts as a diverging lens [27] that shifts the virtual object plane and modifies its magnification to approximately 2/3. Electrons that enter the lens through this opening may be treated as coming from the virtual object along linear trajectories with kinetic energy, E, following acceleration. These electrons are strongly focused by an image forming electrostatic or magnetic lens element that is positioned close to the first electrode in the objective lens. This produces a diffraction pattern in the back focal plane of the lens. An image is formed with electrons that are selected using an angle-limiting contrast aperture in a subsequent diffraction plane in the imaging lens column. The aberrations of the objective lens that affect the fidelity of image formation and information transfer have been studied theoretically by analytical and ray tracing methods and can be measured experimentally [24–26,28]. The size of the contrast aperture likewise affects information transfer and determines the diffraction limit to resolution. An optimum aperture size is chosen that balances contributions to resolution from the diffraction limit that dominate at small acceptance angle and aberrations that dominate at large acceptance angle.

2.2. FO and CTF models

Emitted electrons are described by an object wave, $\psi_o(r) = \sigma(r)\exp(i\phi(r))$, where r is the lateral position, and σ and ϕ are the amplitude and phase of the emitted electron wave, respectively. A point on the object is broadened in the image by the imaging system. This broadening is described by the point spread function, $h(r)$. The full image wave function is therefore obtained by convolution of the object function with the point spread function, $\psi_i(r) = \psi_o(r) * h(r)$. In FO and CTF methods, modifications of the object wave by the microscope are incorporated by their effect on the Fourier transform of the object function, $\Psi(q)$, where the spatial frequency $q = \alpha/\lambda$ is the conjugate variable to the position, α is related to the emission angle from the virtual object and λ is the wavelength of the electron after acceleration to the microscope potential, typically 15–20 kV. In the image plane with magnification M = 1 that the image intensity calculation is conveniently performed, the angle α is a factor of 2/3 smaller than the emission angle from the virtual object due to the demagnification of the virtual object. Using the convolution theorem, the Fourier transform of the image wave function is given by $\widetilde{\Psi}(q) = \Psi(q)H(q)$, where $H(q)$ is the Fourier transform of $h(r)$. $H(q)$ describes how information at different spatial frequencies is transmitted through the microscope. It is called the contrast transfer function and has the separable schematic form

$$H(q) = M(q)W(q, \Delta z)E_C(q)E_S(q, \Delta z)E_{U,I}(q).$$

$M(q)$ is the aperture function that accounts for the angular confinement caused by the contrast aperture. $W(q,\Delta z)$ is the wave aberration function that includes the effects of spherical aberrations and defocus, Δz. E_S is the source extension envelope function that incorporates the effect of the limited spatial coherence due to beam divergence, which is described by the angular spread α_{ill} of the electron illumination. E_C is the chromatic envelope function that accounts for the finite energy spread of the electron source, ΔE, and chromatic aberrations, and $E_{U,I}$ is an envelope function caused by instabilities of the lens current and voltage. E_C and $E_{U,I}$ together describe the temporal coherence of the system. Since the effects of instabilities are negligible in LEEM [18,21], $E_{U,I}$ will no longer be considered here. Expressions for all of the terms have been presented before for uncorrected and aberration-corrected microscopy [18,21]. We address the case of uncorrected microscopy here.

The image intensity is calculated as the absolute square of the image wave function, $I = \psi_i \cdot \psi_i^*$, where the image wave function is the inverse Fourier transform of the modified object Fourier transform, $\psi_i = \mathbb{F}^{-1}\widetilde{\Psi}$. The key difference between FO and CTF approaches is the way in which the image intensity calculation is done. The intensity in an image plane with magnification M = 1 may be written in compact form

$$I(r) = \iint_{q,q'} \Psi(q)\Psi^*(q')R(q, q', \Delta z)\exp\left(i2\pi(q - q')r\right)dqdq',$$

where the cross-coefficient is the absolute square of the contrast transfer function

$$R(q, q', \Delta z) = H(q)H^*(q') \equiv R_0(q, q', \Delta z)E_C(q, q')E_S(q, q', \Delta z),$$

with

$$R_0(q, q', \Delta z) = M(q)M^*(q')W(q, \Delta z)W^*(q', \Delta z),$$

and the terms $E_C(q,q')$ and $E_S(q,q',\Delta z)$ are composite envelope functions, whose forms differ for FO and CTF.

In CTF, the inverse transforms that are carried out to evaluate the image wave function and its complex conjugate are treated independently. This means that the composite envelope functions are

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