Effects of low-spatial-frequency response of phase plates on TEM imaging

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Abstract
Images of simple objects produced by a perfect lens and a phase plate have been calculated by use of Abbe theory for Foucault, Hilbert and Zernike phase plates. The results show that with a Zernike plate, white outlines and ringing like those observed previously can be caused by the beam hole, which limits the low-spatial-frequency response of the system even when the lens behaves perfectly. When the change of phase added by the phase plate is distributed over a range of radius rather than a simple step, the unwanted effects are substantially reduced.

1. Introduction
A phase plate in the back focal plane (BFP) of a TEM objective lens can improve contrast at focus for phase objects but may also produce some unwanted effects. Hilbert plates give an impression of adding shadows to an object or differentiating it [1]. Zernike plates may produce white outlines and sometimes ‘ringing’ of intensity around large objects [2, 3]. Detailed modelling of the response of an objective lens to a single spatial frequency does not show why this behaviour occurs. However, when the effect of a lens and phase plate on an object wave is modelled by including all spatial frequencies and the transverse extent of the object, it becomes clear that the observed defects can be caused by the response of the phase plate to low spatial frequencies, and in particular by its profile closest to the electron beam. The behaviour of interest can be calculated using basic wave-optical theory and with the simple assumption of perfect lens behaviour.

2. Analysis for plate and perfect lens
The image of a physical object depends on more than the contrast transfer function of a single spatial frequency. Such an object contains a spectrum of frequencies and also extends over a transverse area. The image can be found by using Abbe’s theory of imaging [4]:

- The object’s phase distribution \( f(x_o) \) has a spectrum \( F(q) \) in angular spatial frequency \( q \);
- The lens collects rays of the same \( q \) at a single transverse coordinate \( x_p \) (or \( r_p \)) in the BFP;
- The phase plate multiplies the spectrum by a transmission function \( T \) which is a function of \( x_p \) (or \( r_p \)) and so of \( q \) (when the plate is at the BFP);
- The modified spectrum \( T(q)\ F(q) \) is transformed to an amplitude distribution \( g(x_i) \) at the image plane.

The type of transform to be used depends on the geometry of the system. If both the phase distribution of the object and the phase plate geometry can be expressed in Cartesian coordinates (x, y), then Fourier transforms can be used. If both the object and the phase plate can be described in
polar transverse coordinates \((r, \theta)\), then Hankel transforms are needed. The Hankel transform can be found by conversion from the Fourier transform \[5\], replacing \(x_0\) and \(y_0\) by \((r_0 \cos \theta_0)\) and \((r_0 \sin \theta_0)\), and \(q_x\) and \(q_y\) by \((q \cos \theta_p)\) and \((q \sin \theta_p)\). In either coordinate system, if the object and the plate can each be described by a single product of functions of single transverse coordinates, then the general 2D transforms reduce to products of 1D transforms.

In modelling the object phase distribution it is convenient to represent separately the magnitude of the phase variation, written here as \(A\), and its spatial distribution, written as \(\phi(x_0)\) or \(\phi(r_0)\) with a maximum value of 1. The theory here is written for a weak phase object for which \(A \ll 1\). Then the object exit wave \(f\) can be approximated by \([1 + iA\phi(x_0)]\) (with variation as \(\exp i(kz - \omega t)\) omitted). We represent the image wave by a power series in \(A\), of the form \([1 + iA\eta(x_i) + O(A^2)]\), where a function \(\eta\) (as yet unknown) is used because its spatial distribution will be shown to differ from \(\phi\). The image amplitude is proportional to \([1 - A \text{Im}(\eta)]\) to first order, so the intensity is proportional to \([1 - 2A \text{Im}(\eta) + O(A^2)]\). Thus when the direct beam is present at the detector, the range of intensity due to object phase variation is proportional to \(A\). The lens is assumed to be perfect, in the sense of having no aberrations or frequency-dependent phase shift.

3. Types of phase plate

The phase plates considered here are the Foucault (or knife-edge), Hilbert and Zernike plates. For Cartesian geometry as needed for Foucault and Hilbert plates, the object is a strip of width \(2b\) so its phase distribution is \(\phi(x_0) = 1\) for \(|x_0| < b\), 0 for \(|x_0| > b\). The Fourier spectrum of the function \(f(x_0)\) is then \(F(q) = \sqrt{2\pi} \delta(q) + iA\sqrt{2/\pi} \sin qb / q\).

3.1. Foucault plate

This plate is straight-edged and opaque, at a spacing defined as \(q_0\) from the axis of the direct beam. The transmission function of the plate is \(T(q) = 1\) for \(q < q_0\), else = 0. The real part of the image function can be expressed using (tabulated) cosine integral functions \(\text{Ci}\) [6, 7] as \((1 - A I_1 / 2)\), where

\[
I_1(X_i, B) = \left[\text{Ci} [X_1 + B] - \text{Ci} [X_1 - B]\right] / \pi
\]

Here \(X_1 = q_0 x_i\), \(B = q_0 b\) and \(x_i\) is the transverse coordinate in the image plane, measured in the same direction as \(q\). The assumed distribution of phase is even in \(x_0\), but the function \(I_1\) is odd in \(x_i\) so \(I_1\) does not model this object well. When plotted as a function of \(x_i\) or modelled by converting intensity to a monochrome scale (figure 1), \(I_1\) gives the appearance of the derivative of the object function.

3.2. Hilbert plate

The physical layout is as for the Foucault plate, but the Hilbert plate is transparent and adds a phase \(\alpha\) relative to free space, where it is present. Its transmission function is thus

\[
T_2(q/q_0) = \exp i\alpha(q/q_0), \quad \theta = \begin{cases} 0, & 0 < q/q_0 \\ \alpha, & 1 < q/q_0 \end{cases}
\]

The resulting real part of the image function is [8]

\[
\text{Re}(g) = 1 - A \sin \alpha / 2 \left[I_1 \sin \alpha / 2 + I_3 \cos \alpha / 2\right]
\]
where $I_1$ is as defined by (1) and $I_3$ is defined by

$$I_3(X_i, B) = \phi(-X_i/B) - \left[ Si(X_i + B) - Si(X_i - B) \right] / \pi$$

Here $Si(\cdot)$ is the sine integral function defined in [7]. The function $I_3$ is even in $x_i$ (figure 2), but if $\alpha$ is chosen as $(2n\pi)$ to maximise $\cot \alpha/2$, the amplitude variation vanishes to first order. Thus an image from a Hilbert plate is likely to consist partly of function $I_1$ and so does not provide an accurate image of this even object.

3.3. Zernike plate with step phase transition
The rotationally symmetric object considered here is a disc of diameter $2b$ providing a phase change defined as $\phi(r) = 1$ for $r < b$, 0 for $r > b$. This implies a step change in the object phase at $r = b$. A Zernike plate consists of a sheet with a central circular hole, outside which the phase change relative to free space is uniform and typically $\pi/2$. Its effect can be found by Hankel transforms as indicated above and in [6, 8]. The image intensity as a function of radius can be calculated numerically with software such as Mathematica [9], which also provides conversions to area density plots.

The transition in phase at the edge of the central hole in the plate is modelled here first by a simple step at spatial frequency $q_0/2\pi$. Images of disc objects of four sizes are shown in figure 3.

![Figure 3](image.png)

**Figure 3.** Step phase change introduced by a Zernike plate at the beam hole, and resulting image functions for circular phase objects of (dimensionless) radii $B = q_0b = 1, 2, 4$ and 8. The colour level of 0.5 at the image corresponds to zero phase added by the object.

Disc objects of size $B \leq 1$ are imaged well, but the images of larger objects show radial fluctuations of amplitude that are not present in the object phase. Also the image function of figure 3, like that of figure 2, models the step change in the phase added by the object, $\phi(r)$ at $r = b$, by a change from 0.5 to 1 for $B \ll 1$ but by a step from 0.25 to 0.75 for larger objects. The fluctuation of image amplitude with radius is continuous except at the step, but is depressed at radii near and on both sides of the step. The most obvious effect is a brightening of the image outside the step over a range of radii of $q_0\Delta r \sim 2$, which appears to correspond to the white outlines reported earlier [2].

3.4. Zernike plate with broadened phase transition
The radial fluctuations in image amplitude generated when there are sharp transitions in both the object phase and the phase-plate transmission resemble the fluctuations or ‘ringing’ that can appear when an electronic amplifier with sharply-varying frequency response is used to amplify a square wave. These effects in an amplifier can be reduced by broadening the frequency response, so the calculations for a Zernike plate were modified by broadening the range of $q$ over which its phase...
transition occurred. The results are shown in figure 4 for three transitions. In each case, half the total phase change occurs at \( q = q_0 \).

4. Conclusions
A Foucault plate or a Hilbert plate whose phase shift \( \alpha \) is an odd multiple of \( \pi \) will, even with a perfect lens, produce an odd image distribution. Then the image of a rectangular weak phase object resembles a spatial derivative of the object phase. If \( \alpha \) for a Hilbert plate has some other value, the image will include an even function together with the odd function, but as \( \alpha \to 2\pi n \) the contrast at focus falls to zero.

A Zernike plate can image phase objects more accurately but, with a step change in phase at the beam hole, the intensity for objects with \( B > 1 \) fluctuates with radius. The fluctuation can be reduced by making the phase change occur over a broader range of radii, for instance by use of a ferromagnetic ring. The plate may add white outlines to large objects, resulting from the limitation of phase shift at radii near the direct beam radius, but is still able to provide the desired increase in phase contrast at exact focus.

References
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Figure 4. Plots of \( \theta(q/q_0) \) and of image function for \( \alpha = \pi/2 \) and \( B = q_0, b = 1, 2, 4 \) and 8, for three distributions of phase added near the centre of a Zernike plate. The radial and colour scales for the image function are as for Fig. 3.