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Application of Rigorous Numerical Techniques to the Calculation of Images in Scanning Optical Microscopy

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The standard approach to describe the process of image formation in optical microscopy is based on scalar wave theory and on approximate models for describing the interaction of the optical field with the structure of the object. The validity of this approach becomes questionable when the object contains features comparable to the wavelength, and when the structures are optically thick.

In this work, we consider the problem of image formation in scanning optical microscopy. Under the assumption that the sample is one-dimensional and assuming also a one-dimensional optical system, we have developed a fairly rigorous approach to describe the image formation process. By one dimensional we mean a sample whose properties, when referred to a cartesian coordinate system, may present changes along, say, the x direction and are constant along the y one. We divide the process of image formation in the scanning optical microscope into three parts: We first need a mathematical description of the field incident on the sample. In the second stage, we need an accurate model to describe the interaction between this field and the sample. This is essentially a scattering problem, and there is no simple way of solving problems of this kind. The main feature of our work is that this aspect of the problem is approached in a fairly rigorous manner. In the third stage, the reflected light is propagated back through the optical system toward the detector. The angular size and position of the detector can be rather arbitrary and in fact define the mode of image formation. The image is formed on a point-by-point basis by scanning the sample under this point spread function. Various modes of image formation have been considered, including coherent, partially coherent, dark field and confocal. The sample is normally assumed to be a surface relief object ruled on a homogeneous material characterized by its complex refractive index, but calculations with layered objects have also been performed.

To illustrate the method, and for brevity, we restrict the discussion here to the case of a perfectly conducting surface illuminated by s-polarized light. As mentioned, we first need to provide an adequate description of the beam incident on the surface. For an s-polarized beam the only non-zero component of the electric field is its y component. We assume that the lens is diffraction limited and, thus, that the complex amplitude associated with the incident field on the plane z=0 is a “sinc” function. This in-cident field is propagated to out-of-focus planes using angular spectrum techniques. It results in the following expression (Aguilar and Méndez, 1994):

$$E_i(u,v)=\exp[-i(\frac{u}{\alpha_m^2}+\frac{v^2}{2u})]\sqrt{\frac{\pi}{4u}}\,[f(\sqrt{\frac{u}{\pi}}+\frac{v}{\sqrt{u\pi}})+f(\sqrt{\frac{u}{\pi}}-\frac{v}{\sqrt{u\pi}})], \tag{1}$$

where

$$f(x)=\int_0^x \exp(i\frac{\pi}{2}\xi^2)\,d\xi, \tag{2}$$

the optical coordinates v and u are given by

$$u=k\alpha_m^2 z,$$
$$v=k\alpha_m^2 x,$$

$k=2\pi/\lambda$ is the wavenumber, and the constant α_m

represents the numerical aperture of the system.

Due to our assumptions, after interacting with the surface, the field remains s polarized, and this simplifies matters considerably; throughout the whole process of image formation we then only have to deal with the y component of the electric field. The surface profile is represented by the function $z=\zeta(x)$, and using Green's integral theorem, one can express the total field above the surface as the sum of the incident and scattered fields:

$$E(x,z)=E_i(x,z)+\frac{1}{4i}\int_{-L/2}^{L/2} H_0^{(1)}(k[(x-x')^2 +(z-\zeta(x))^2]^{1/2})F(x')dx', \qquad (3)$$

where

$$F(x')=[-\zeta'(x')\frac{\partial}{\partial x'}+\frac{\partial}{\partial z'}]E(x',z'). \qquad (4)$$

Here, $H_0^{(1)}$ represents a Hankel function of the first kind and order zero, and L represents the length of the surface. The second term on the right hand side of Eq. (3) represents the scattered field, which is determined by the source function F(x), related to the normal derivative of the field on the surface.

By taking the limit $(x,z) \to [x_0,\zeta(x_0)]$, and using the fact that the total electric field on the surface must vanish, it is possible to write an integral equation that determines the source function F(x). We find that

$$E_i(x_0)=\lim_{\eta\to 0}\int_{-L/2}^{L/2} L_0(x_0,x',\eta)F(x')dx', \qquad (5)$$

where

$$L_0(x_0,x',\eta)=-\frac{1}{4i}\int_{-L/2}^{L/2} H_0^{(1)}(k[(x-x')^2 +(z-\zeta(x))^2]^{1/2})F(x')dx', \qquad (6)$$

with $\eta>0$.

The integral equation expressed by Eq. (5) was first converted into a matrix equation and then, to find F(x), the matrix equation was solved employing standard numerical techniques. The intensity reaching the detector can then be calculated for a given geometry. This provides the signal associated with a particular position of the surface along the x direction.

Rigorous images can be calculated in this fashion. Effects such as multiple scattering and changes in the state of polarization of the scattered light are taken into account. We have found that for steplike objects the Kirchhoff approximation gives images that are in good agreement with those obtained with the integral equation approach. A similar conclusion has been reached for the case of ridgelike structures. However, for the case of groovelike structures, multiple scattering is possible and this makes the Kirchhoff approximation inadequate to describe the image formation process. This effect is more pronounced in partially coherent modes of image formation.

The confocal scanning optical microscope, with its depth discrimination property, can also be used to estimate the profile of highly reflecting samples. In the profilometer mode of operation the sample is scanned along the z direction, and the position at which the maximum intensity is reached is associated with the relative height of the surface at that particular position of the sample along the x axis. For this case, we have found that the instrument can successfully estimate a given surface profile when:

i) - The local surface slope does not exceed a given maximum value.

ii) - The surface can be considered locally flat.

Concerning the first statement, we have proposed a criterion for the upper limit in the local slope. The second conclusion implies that the lateral resolution of the instrument is much worse when used as a profilometer than when used as an imaging system. It is also worth mentioning that unresolved features introduce spurious details in the estimated profile.

REFERENCES

Aguilar JF, ER Méndez. 1994. Imaging optically thick objects in scanning microscopy: perfectly conducting surfaces. J. Opt. Soc. Am. **A 11:** 155-167.