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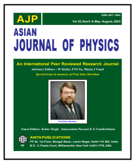

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Modeling of images of patterned dielectric layers on a substrate: A review

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Dedicated in memory of Prof John Sheridan

We review modeling of image formation in the reflection geometry of dielectric structures. Early work on applying rigorous scattering theory to image modeling was reported by John Sheridan, in his doctoral thesis. He also investigated approximate methods for scattering calculations. More recent developments in approximate methods based on Born or Kirchhoff approximations are also reviewed. These can be applied to image modeling and reconstruction in partially coherent, confocal or interferometric systems, including low-coherence interference microscopes.

Keywords: Gratings, Diffraction, Scattering, Image formation, Metrology.

1 Introduction

This paper is a tribute to John (Sean) Sheridan. John received his D Phil degree from the University of Oxford, for research into diffraction by volume hologram gratings. His main supervisor was Laszlo Solymar, with whom he worked mainly on diffraction by stacked gratings. I was his secondary supervisor, and he also worked with me on modeling of image formation based on scattering theory, where his expertise in rigorous diffraction theory was fundamental. The present paper is a review of the modeling of patterned, thick, dielectric layers on a substrate, as occur in semiconductor wafer technology. If the spatial wavelength of the patterning is large, then images of isolated edges, lines or grooves can be simulated.

2 Imaging theory

Our first publication together was a conference paper, in 1989 [1]. This presented our general approach, which was to model imaging by an angular spectrum approach. The grating is taken in the x-z plane, independent of the y coordinate. Skew waves were neglected. The sample is illuminated by a plane wave, which scatters with a scattering function $s(\theta_1, \theta_2)$. The angular spectrum $A(\theta_1, \theta_2)$ detected is

$$A(\theta_1, \theta_2) = P_1(\theta_1)\exp\{ ik[x(\sin\theta_2 - \sin\theta_1) + z(\cos\theta_1 + \cos\theta_2)]\} \times s(\theta_1, \theta_2)\, P_2(\theta_2) \quad (1)$$

Here, $P_1(\theta_1)$, $P_2(\theta_2)$ are the strengths of the illuminating wave and the detection sensitivity, respectively, given by the pupil function of the illuminating and detection lenses. For an aplanatic system, these include the aplanatic factors $\cos^{1/2}(\theta_{1,2})$. Then an image is generated by integrating over the pupil functions. For conventional coherent imaging, the illuminating pupil function degenerates to a delta function. For conventional partially-coherent imaging, the amplitude is integrated over the imaging lens pupil, and the intensity is integrated over

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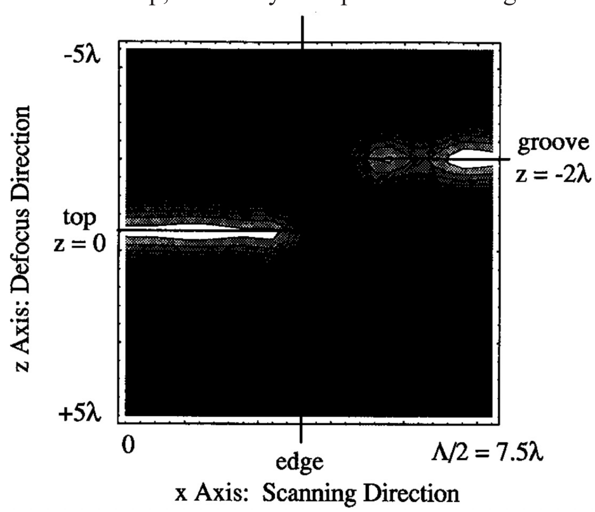
the condenser lens pupil. For a partially-coherent scanning system system, the amplitude is integrated over the illuminating pupil, and the intensity is integrated over the pupil of the collection lens. From the symmetry of Eq (1), if the scattering function obeys reciprocity, as it usually does, then these two partially-coherent systems behave equivalently. For a confocal system, the amplitude is integrated over the two pupils, and finally the image intensity calculated from the squared modulus. In-focus and defocused confocal images were presented for TE polarization, calculated using the rigorous modal method [1]. A number of different approximate methods were investigated, and these were investigated further in Refs [2-4]. In a later paper, coherent brightfield and darkfield imaging of isolated, narrow, line and groove structures in the dielectric layer was investigated [5]. In a further paper, coherent brightfield, coherent darkfield and confocal images of a step edge, and the edge of a dielectric layer, were plotted, and are reproduced below (Fig 1) [6]. It is seen that the brightfield and darkfield images (top right and bottom left) are difficult to interpret. However, the confocal image of the step edge (numerical aperture NA = 0.666) (top left) shows a bright in-focus reflection from the surface on both sides of the step, caused by the optical sectioning effect of confocal imaging.



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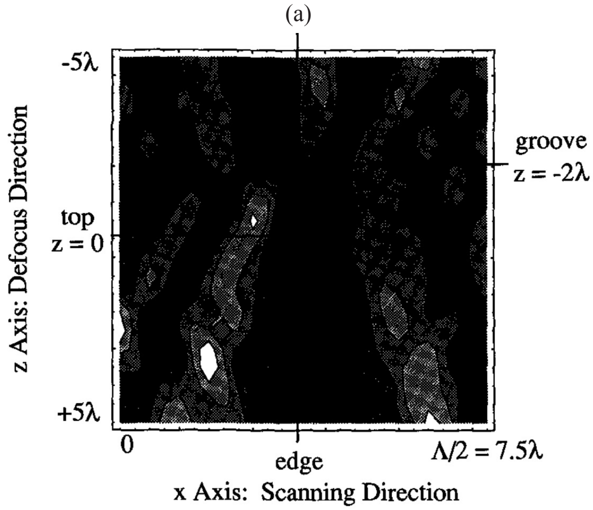

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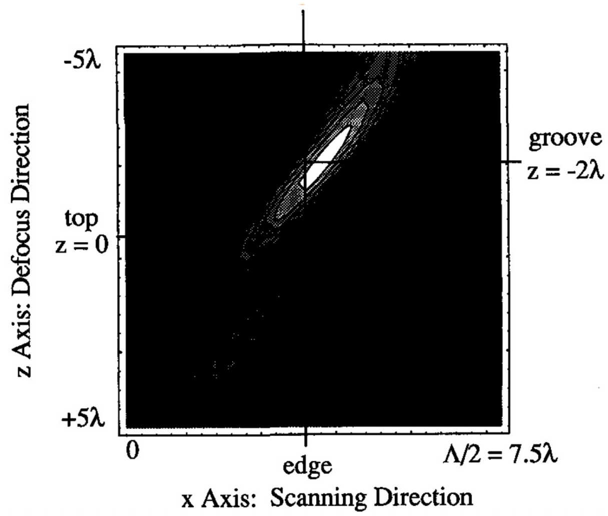

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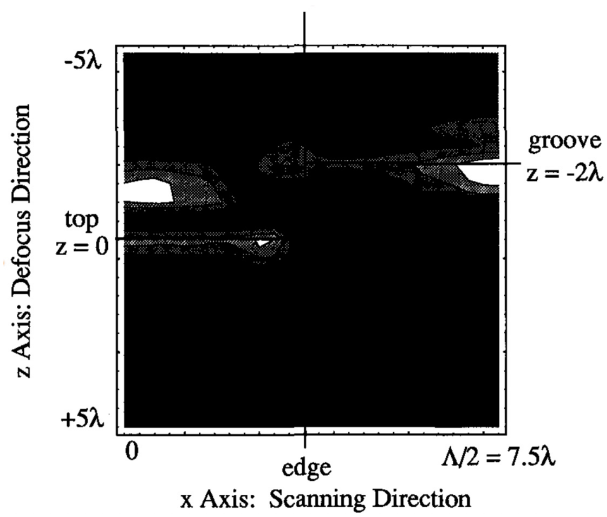

(d)

Fig 1. Top left: Confocal image of a step edge, $n = 4$, thickness 2λ. NA = 0.666. Top right: Coherent bright field image of the edge of a dielectric layer, $n = 1.5$, thickness 2λ, on a substrate, $n = 4$. NA = 0.866. Bottom left: Coherent dark field image of the dielectric edge. Bottom right: Confocal image of the dielectric edge. Note that vertical height is plotted downwards. Reproduced with permission from [6]. Copyright Elsevier Science B.V. ,1994.

The image of the bottom of the edge (labelled groove) suffers from strong shadowing effects. The confocal image of a dielectric layer on a substrate (bottom right) shows in-focus reflection both from the surface and from the interface with the substrate. The reflection from the interface is offset relative to that from the bare substrate (labelled groove), as a result of distortion by the different refractive index of the dielectric, relative to the substrate. As the diffraction theory used is rigorous, it incorporates the effect of spherical aberration caused by imaging through the layer.

3 Alternative scattering theories

The angular spectrum imaging approach can be used with different rigorous scattering theories, including modal and coupled wave theories [7-9]. In general, scattering is a function of four variables, two spatial frequencies to describe the directions of the incident and scattered waves, respectively. The angular spectrum approach to diffraction imaging was perhaps first investigated by Stokes [10]. Wolf went on to propose using an approximation based on the first Born approximation, leading to a solution of the inverse problem [11]. The object function is called the scattering potential. The three-dimensional (3D) Fourier transform (FT) of the scattering potential is also 3D, unlike the scattering function, which is 4D. Nyyssonen applied the angular spectrum method to imaging of grating structures in a nearly coherent system using a modal method [12]. She neglected evanescent wave components in her model, which we found were necessary to ensure convergence, even though these components are not detected. Further developments considered layers with shaped edge profiles, and effects of polarization [13,14].

The simplest model for a surface structure or dielectric layer treats the object as a two-dimensional phase screen. A surface step is represented by a change in phase. For a dielectric layer, reflections from the top and bottom surfaces interfere to result in an effective reflectivity and phase. But this model is only useful if the thickness of the sample is small compared with the depth of focus of the optical system. An improvement is to take account of the defocus at each surface and to use superposition [15]. For systems with high numerical aperture, it is important to express defocus as *kz , relative to the substrate* $\cos\theta$, rather than the paraxial forms $(1-\theta^2/2)$ or $kz[1-(\sin^2)/2]$ [16]. It was shown that for a surface step, there are topologically very few different behaviours that are possible, one of which gives rise to the well-known 'bat wing' surface profile [17].

Instead of using scattering angles, they can be written in terms of lateral and axial spatial frequencies, m, s [18].

$$\tilde{m} = \lambda m = \sin\theta_2 - \sin\theta_1$$

$$\tilde{s} = \lambda s = \cos\theta_1 + \sin\theta_2$$

Here the tildes represent normalized spatial frequencies. These can be generalized to the full 3D case, where θ, ϕ are spherical polar coordinates. For each lens we have:

$$\tilde{m}_1 = \lambda m_1 = \sin\theta_1 \cos\phi_1,\ \tilde{m}_2 = \lambda m_2 = \sin\theta_2 \cos\phi_2$$

$$\tilde{n}_1 = \lambda n_1 = \sin\theta_1 \sin\phi_1,\ \tilde{n}_1 = \lambda n_2 = \sin\theta_2 \sin\phi_2$$

$$\tilde{s}_1 = \lambda s_1 = \cos\theta_1,\ \tilde{s}_2 = \lambda s_2 = \cos\theta_2$$

Thus for the spatial frequencies in the image,

$$\tilde{m} = \lambda m = \sin\theta_2 \cos\phi_2 - \sin\theta_1 \cos\phi_1$$

$$\tilde{n} = \lambda n = \sin\theta_2 \sin\phi_2 - \sin\theta_1 \sin\phi_1$$

$$\tilde{s} = \lambda s = \cos\theta_1 + \cos\theta_2$$

It is seen that for the 3D case, scattering in general is $(\theta_1, \phi_1; \theta_2, \phi_2)$, but the spatial frequencies m, n, s in the image are 3D.

Another interesting case is the rigorous confocal image of a simple dielectric layer on a reflecting substrate. Multiple reflections occur in the Fabry-Perot structure, giving rise to a series of axial peaks, rather than just two reflections from the two surfaces [19,20]. Again, depth distortion and spherical aberration are incorporated into the model, which also incorporates polarization effects. Confocal imaging of a medium with axially varying refractive index was investigated [21]. If the variations in refractive index are weak, equivalent to neglecting multiple scattering, the reflection coefficient can be calculated as a function of angle of incidence. This approach to calculation of the reflection coefficient from a multi-layer stack was further considered [22]. The predictions agreed very well with exact calculations. This model for the reflection coefficient gives an alternative to the Born approximation of Wolf, which is effectively based on the Kirchhoff approximation.

The Kirchhoff approximation can also be used to calculate scattering by a surface profile structure, and therefore also its image in a confocal or interferometric system, valid if surface slopes are small and shadowing effects can be ignored [22,23]. This approach leads to a scattering potential that is different from that based on the Born approximation, but its FT is still 3D, rather than the rigorous 4D scattering theories. A polarization model can be applied to 3D variations in refractive index, if these are weakly changing [24, 25]. This scattering potential is more appropriate than that based on the Born approximation for imaging in a reflection geometry. In this model, scattering occurs as a result of changes in refractive index, rather than the absolute value of the refractive index in the Born approximation. The scattering potential for the Born approximation is proportional to $(n^2 - n_0^2)$, while for the Kirchhoff approximation it is proportional to $-(\nabla^2 \ln n)/4k^2$ [25].

The approach can be applied to scattering and image formation by random surfaces [26]. The Kirchhoff scattering potential was reviewed in Refs [26,27], and has recently been used to model imaging in low-coherence interference systems [28].

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He is elected Fellow of OSA, SPIE, IEE, Institute of Physics, Japan Society for Applied Physics, and the Royal Microscopical Society. He served as Vice-President of the International Commission for Optics (ICO), and as President of the International Society for Optics Within Life Sciences (OWLS). He was awarded the Italian Society for Optics and Photonics Galileo Galilei Medal, Institute of Physics Optics and Photonics Division Prize, Max Planck Bonhöffer Medal, Humboldt Research Award, ISATA Mercedes Award, National Physical Laboratory Metrology Award, Prince of Wales Award for Industrial Innovation, British Technology Group Academic Enterprise Award, and the IEE Gyr and Landis Prize.

He developed an early laser microscope (1975), patented scanning microscopy using Bessel beams (1977), published the first demonstration of scanning two-photon microscopy (by SHG) (1977), published the first paper on Bessel-Gauss beams (1978), proposed two-photon fluorescence and CARS microscopy (1978), launched the first commercial confocal microscope (1982), developed the first confocal microscope with computer control and storage (1983), proposed scanning microscopy using a detector array with pixel reassignment, now known as image scanning microscopy (1988). He has made substantial contributions in the fields of diffraction theory, beam propagation, pulse propagation, scattering and inverse scattering, image formation, and polarization algebra.