Complex pupil function reconstruction at high numerical aperture using the extended Nijboer-Zernike diffraction theory

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ABSTRACT

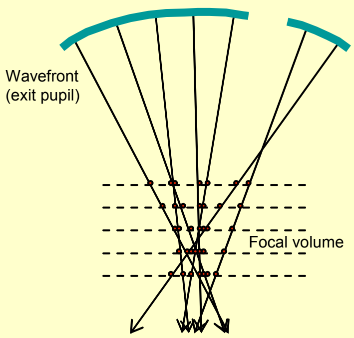
We have derived an analytical expression for the field components in the focal region of a high-numerical-aperture imaging system using the so-called Extended Nijboer-Zernike diffraction theory. It is shown that the transmission function, aberrations and polarization properties of an imaging system with high numerical aperture can be derived from the through-focus intensity map via an inversion process based on this analysis.

Problem definition:

How to retrieve optical system properties (*amplitude, phase and* polarization in the exit pupil) from *intensity* measurements through the *focal volume*?

1) *Intuitive picture*

(based on ray optics)

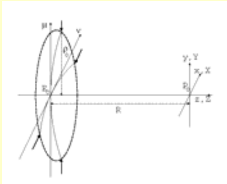


Ray density variation in the focal volume due to wavefront aberration *and* transmission variation

2) *Scalar imaging*

Analytic 'tool' derived from the Extended Nijboer-Zernike theory, first developed for the scalar imaging case ('point source')

$$U(r,\varphi;f)=\frac{1}{\pi}\int_0^1 \rho\exp(if\rho^2)\int_0^{2\pi} A(\rho,\vartheta)\exp\{i\Phi(\rho,\vartheta)\}\exp\{i2\pi r\rho\cos(\vartheta-\varphi)\}d\vartheta d\rho$$



Exit pupil and focal volume: co-ordinates

Introduction of Zernike polynomial expansion representing amplitude *and* phase:

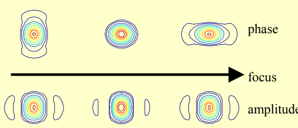
$$A(\rho,\vartheta)\exp\{i\Phi(\rho,\vartheta)\}=\sum_{n,m}\beta_n^m R_n^{|m|}\exp(im\vartheta)$$

Semi-analytic solution, see A.J.E.M. Janssen, J. Opt. Soc. Am **A19**, 849-857 (2002):

$$U(r,\varphi;f)=2\sum_{n,m} i^m\beta_n^m V_n^m(r,f)\cos m\varphi \qquad V_n^m(r;f)=\int_0^1 \rho\exp(if\rho^2)R_n^m(\rho)J_m(2\pi r\rho)d\rho$$

$$V_n^m(r;f)=\exp(if)\sum_{l=1}^{\infty}(-2if)^{l-1}\sum_{j=0}^{p} v_{lj}\frac{J_{m+l+2j}(v)}{lv^l};\ p=(n-m)/2,\ v=2\pi r$$

$$v_{lj}=(-1)^p(m+l+2j)\binom{m+j+l-1}{l-1}\binom{j+l-1}{l-1}\binom{l-1}{p-j}\Big/\binom{q+l+j}{l};\quad q=(n+m)/2$$



Through-focus intensity map for a second-order phase aberration (astigmatism; upper figure) and a quadratic transmission defect (lower figure)

3) *Vectorial imaging*

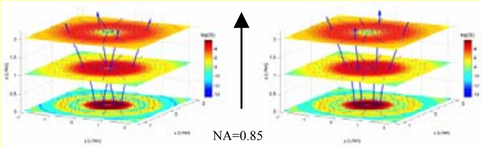
Complication in a high NA imaging system: *vectorial* calculation of the aberrated intensity distribution is needed in the focal volume !

Electric field density in the focal volume is given by $w_E=\frac{\varepsilon_0}{4}n_r^2|E|^2=\frac{\varepsilon_0}{4}n_r^2\{E_1E_1^*+E_2E_2^*+E_3E_3^*\}$

The electric field vector produced by a point source illuminating an aberrated optical system (complex pupil function given by *two* sets of Zernike coefficients $\beta_n^{m,x}$, $\beta_n^{m,y}$) is given by

$$\vec{E}^x(r,\varphi;f)=-i\gamma s_0^2\exp\left(\frac{-if}{1-\sqrt{1-s_0^2}}\right)\sum_{n,m} i^m\beta_n^{m,x}\exp(im\varphi)\begin{pmatrix} V_{n,0}^m+\frac{s_0^2}{2}V_{n,2}^m\exp(2i\varphi)+\frac{s_0^2}{2}V_{n,-2}^m\exp(-2i\varphi)\\ -\frac{is_0^2}{2}V_{n,2}^m\exp(2i\varphi)+\frac{is_0^2}{2}V_{n,-2}^m\exp(-2i\varphi)\\ -is_0V_{n,1}^m\exp(i\varphi)+is_0V_{n,-1}^m\exp(-i\varphi)\end{pmatrix}$$

see: J.J.M. Braat, P. Dirksen, A.J.E.M. Janssen, A.S. van de Nes, J. Opt. Soc. Am. **A20**, 2281-2292 (2003)



Vectorial *forward* calculation using the semi-analytic Extended Nijboer-Zernike theory
Energy flow (arrows) and intensity distribution (colour coded) in the focal region;
Left: circularly polarized Right: circularly polarized + orbital angular momentum

Energy density in the focal region

$$\beta_n^{m,x}=a\beta_n^m;\quad \beta_n^{m,y}=b\beta_n^m;\quad (|a|^2+|b|^2=1 \text{ for normalisation purposes})$$

$$w_E(r,\varphi;f)=\frac{\varepsilon_0 n_r^2 s_0^2}{4}\begin{bmatrix} G_{00}(\beta,\beta)+\\ s_0^2\left\{\left[|a|^2-|b|^2\right]\mathrm{Re}\{G_{0,2}(\beta,\beta)\}-2\,\mathrm{Re}(ab^*)\,\mathrm{Im}\{G_{0,2}(\beta,\beta)\}\right\}+\\ s_0^2\left\{\left[|a|^2-|b|^2\right]\mathrm{Re}\{G_{0,-2}(\beta,\beta)\}+2\,\mathrm{Re}(ab^*)\,\mathrm{Im}\{G_{0,-2}(\beta,\beta)\}\right\}+\\ \frac{s_0^4}{2}\left\{\left[1-2\,\mathrm{Im}(ab^*)\right]G_{2,2}(\beta,\beta)+\left[1+2\,\mathrm{Im}(ab^*)\right]G_{-2,-2}(\beta,\beta)\right\}+\\ s_0^2\left\{\left[1-2\,\mathrm{Im}(ab^*)\right]G_{1,1}(\beta,\beta)+\left[1+2\,\mathrm{Im}(ab^*)\right]G_{-1,-1}(\beta,\beta)\right\}+\\ -2s_0^2\left\{\left[|a|^2-|b|^2\right]\mathrm{Re}\{G_{+1,-1}(\beta,\beta)\}+2\,\mathrm{Re}(ab^*)\,\mathrm{Im}\{G_{+1,-1}(\beta,\beta)\}\right\}\end{bmatrix}$$

$$G_{kl}(\alpha,\beta)=$$
$$\sum_{n,m} i^m\alpha_n^m V_{n,k}^m\exp(im\varphi)\exp(ik\varphi)\times\sum_{n',m'} i^{-m'}\beta_{n'}^{m'}V_{n',l}^{m'*}\exp(-im'\varphi)\exp(-il\varphi)=$$
$$\sum_{n',m'}\exp\{i(m-m')\pi/2\}\exp\{i(m-m'+k-l)\varphi\}\alpha_n^m\beta_{n'}^{m'*}V_{n,k}^m(r,f)V_{n',l}^{m'*}(r,f)$$

Small β_n^m-approximation (dominating β_0^0-coefficient)

$$G_{kl}(\alpha,\beta)=e^{i(k-l)\varphi}\sum_{\nu=0}^{\nu_{\max}}\sum_{\mu=-\mu_{\max}(\nu)}^{+\mu_{\max}(\nu)}\left\{\begin{array}{l} e^{-i\mu\pi/2}e^{-i\mu\varphi}\alpha_0^0\beta_\nu^{\mu*}V_{0,k}^0(r,f)V_{\nu,l}^{\mu*}(r,f)+\\ (1-\varepsilon_{\nu\mu})e^{+i\mu\pi/2}e^{+i\mu\varphi}\alpha_\nu^\mu\beta_0^{0*}V_{\nu,k}^\mu(r,f)V_{0,l}^{0*}(r,f)\end{array}\right\}$$

Conclusions

1)
A parametric analytic expression has been found for the electric field *and* the energy density in the focal volume of an optical system including pupil aberrations, pupil transmission variations and spatially varying birefringence of the imaging system (small source point, high NA)

2)
Complex Zernike coefficients (two sets) are suitable to describe the generalized state of polarization in the exit pupil of the optical system

3)
The *inverse* problem can be solved using a through-focus intensity map (energy density function) to solve a system of linearized equations in the two unknown sets of Zernike coefficients

4)
The extended Nijboer-Zernike analysis offers an eigenfunction expansion for the vectorial propagation operator from exit pupil to image volume. This property can be exploited for the fast *forward* calculation of the image intensity in the focal volume

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