

Trieste, 04.10.2016

Fast physical optics modelling of x-ray systems

Frank Wyrowski, University of Jena & Wyrowski Photonics UG Antonie Verhoeven, University of Eastern Finland Christian Hellmann, Wyrowski Photonics Mourad Idir, BNL

Jena, Germany



My Three Teams at ...

- Applied Computational Optics Group at Friedrich Schiller University of Jena
 - R&D in optical modeling and design with emphasis on physical optics.
- Wyrowski Photonics
 - Development of fast physical optics software VirtualLab Fusion

LightTrans

- Distribution of VirtualLab, together with distributors worldwide
- Service, technical support, seminars, and trainings
- Optical engineering projects











System Modeling Example #1 Provided by Mourad Idir, BNL

- Source
 - $\lambda = 0.1$ nm, 12 keV
 - Spherical wave, fully coherent field
 - 50 m to mirror,12 µrad opening angle
- Mirrors
 - Elliptical, focal points at source & focal plane
 - Gracing angle: $\theta = 3 \text{ mrad}$





System Modeling Example #2 Provided by Mourad Idir, BNL



- **Source modeling:** Representation of source field in input plane of system by set of monochromatic, fully coherent source field **modes**.
- The representation of source fields by modes enables modeling of
 - Fully coherent source fields
 - Partially spatially coherent source fields
 - Partially temporally coherent source fields
 - Ultrashort pulsed source fields
- Electromagnetic source field modes are determined by six field components of the **E** and **H**-field. That includes automatically
 - Energy quantities
 - Wavefront (phase)
 - Polarization
 - Degrees of coherence and polarization
 - Pulsed field characteristics

- **Source modeling:** Representation of source field in input plane of system by set of monochromatic, fully coherent source field **modes**.
- The representation of source fields by modes enables modeling of
 - Fully coherent source fields
 - Partially spatially coherent source fields
 - Partially temporally coherent source fields
 - Ultrashort pulsed source fields



- **Source modeling:** Representation of source field in input plane of system by set of monochromatic, fully coherent source field **modes**.
- The representation of source fields by modes enables modeling of
 - Fully coherent source fields
 - Partially spatially coherent source fields
 - Partially temporally coherent source fields
 - Ultrashort pulsed source fields



- **Source modeling:** Representation of source field in input plane of system by set of monochromatic, fully coherent source field **modes**.
- The representation of source fields by modes enables modeling of
 - Fully coherent source fields
 - Partially spatially coherent source fields
 - Partially temporally coherent source fields
 - Ultrashort pulsed source fields



System Modeling Example #1 Provided by Mourad Idir, BNL

- Source
 - $\lambda = 0.1$ nm, 12 keV
 - Spherical wave, fully coherent field
 - 50 m to mirror,12 µrad opening angle
- Mirrors
 - Elliptical, focal points at source & focal plane
 - Gracing angle: $\theta = 3 \text{ mrad}$

Source





One spherical field mode with 12 µrad opening angle

System Modeling Example #2 Provided by Mourad Idir, BNL



 For extended, quasihomogeneous sources like LED and synchrotron radiation the elementary shifted mode concept is reasonable.

Finite-elementary-source model for partially coherent radiation

Pasi Vahimaa and Jari Turunen University of Joensuu, Department of Physics, P.O. Box 111, FI-80101 Joensuu, Finland pasi.vahimaa@joensuu.fi

P. Vahimaa and J. Turunen, *Opt. Express* **14**, 1376–1381 (2006).

2004 J. Opt. Soc. Am. A/Vol. 27, No. 9/September 2010

Tervo et al.

Shifted-elementary-mode representation for partially coherent vectorial fields

Jani Tervo,^{1,*} Jari Turunen,¹ Pasi Vahimaa,¹ and Frank Wyrowski²

¹University of Eastern Finland, Department of Physics and Mathematics, P.O. Box 111, FI-80101 Joensuu, Finland ²Friedrich Schiller University of Jena, Department of Applied Physics, D-07745 Jena, Germany *Corresponding author: jani.tervo@joensuu.fi

 For extended, quasihomogeneous sources like LED and synchrotron radiation the elementary shifted mode concept is reasonable.



 For extended, quasihomogeneous sources like LED and synchrotron radiation the elementary shifted mode concept is reasonable.



System Modeling Example #2 Provided by Idir Mourad, BNL



 For extended, quasihomogeneous sources like LED and synchrotron radiation the elementary shifted mode concept is reasonable.



- **Source modeling:** Representation of source field in input plane of system by set of monochromatic, fully coherent source field **modes**.
- The representation of source fields by modes enables modeling of
 - Fully coherent source fields
 - Partially spatially coherent source fields
 - Partially temporally coherent source fields
 - Ultrashort pulsed source fields
- Pulses are modeled by a Fourier decomposition of the temporal function, which results in a set of mutually coherent monochromatic source field modes.
- VirtualLab provides 3D modeling of any type of laterally and temporally pulsed field shape.

Physical Optics Modeling: System

- **Source modeling:** Representation of source field in input plane of system by set of monochromatic, fully coherent fields.
- **System modeling:** Sequential or non-sequential propagation of source field modes through system including
 - Free-space propagation
 - Mirrors and lenses; any type of smooth surfaces
 - Surfaces with multilayered stacks
 - Gratings
 - Surfaces with microstructured stacks, e.g. Zone plate
 - Capillary optics
 - ... and whatever component the application might require



VirtualLab enables to tackle all those physical optics modeling challenges!

Physical Optics Modeling: System

- **Source modeling:** Representation of source field in input plane of system by set of monochromatic, fully coherent fields.
- **System modeling:** Sequential or non-sequential propagation of source field modes through system including
 - Free-space propagation
 - Mirrors and lenses; any type of smooth surfaces
 - Surfaces with multilayered stacks
 - Gratings
 - Surfaces with microstructured stacks, e.g. Zone plate
 - Capillary optics
 - ... and whatever component the application might require

Physical optics modeling is considered to be slowly compared to ray tracing. Is that really true?

Basic Modeling Situation



Basic Modeling Situation



Propagation by FFT Techniques



Propagation by FFT Techniques



Propagation by FFT Techniques



Basic Modeling Situation: Boundary Problem



Geometric Field Tracing through Surface



Surface between two media

- Input field is decomposed into local plane wave fields.
- That is theoretically justified if field is in its geometric zone.
- Local plane waves (smart rays) are propagated through surface by local application of plane wave/plane surface interaction (law of refraction and Fresnel's equations).
- By including all vectorial effects and considering intensity law of geometrical optics the output field can be constructed.

Paraxial Modeling of Surfaces



Surface between two media

- In paraxial optics the local plane waves propagate all along the axis and the deflection at the surface by refraction is neglected.
- Then just the optical path length is considered and a phase term proportional to the height profile is obtained.
- That is the thin element approximation (TEA) frequently used in paraxial optics, e.g. Fourier and laser optics.
- Together with Fresnel integral for freespace propagation the Collins integral follows for lens systems.

Fast Physical Optics Modeling



Fast Physical Optics Modeling



Spherical Wave: f = 200 mm; z= 0 - 400mm

Field propagated along the z-axis



Spherical Wave: f = 200 mm; z= 180 – 220 mm

Field propagated along the z-axis



Spherical Wave: f = 200 mm; z= 193 – 207 mm

Field propagated along the z-axis



Spherical Wave: Geometric Zone?

Field propagated along the z-axis



Fast Physical Optics Modeling: Example



Fast Physical Optics Modeling



Geometrical Optics of Electromagnetic Fields

Principles of Optics

7th (expanded) edition

Max Born and Emil Wolf

Electromagnetic Theory of Propagation, Interference and Diffraction of Light

III

Foundations of geometrical optics

3.1 Approximation for very short wavelengths

THE electromagnetic field associated with the propagation of visible light is characterized by very rapid oscillations (frequencies of the order of 10^{14} s⁻¹) or, what amounts to the same thing, by the smallness of the wavelength (of order 10^{-5} cm). It may therefore be expected that a good first approximation to the propagation laws in such cases may be obtained by a complete neglect of the finiteness of the wavelength. It is found that for many optical problems such a procedure is entirely adequate; in fact, phenomena which can be attributed to departures from this approximate theory (socalled diffraction phenomena, studied in Chapter VIII) can only be demonstrated by means of carefully conducted experiments.

The branch of optics which is characterized by the neglect of the wavelength, i.e. that corresponding to the limiting case $\lambda_0 \rightarrow 0$, is known as geometrical optics,* since in this approximation the optical laws may be formulated in the language of geometry. The energy may then be regarded as being transported along certain curves (light rays). A physical model of a pencil of rays may be obtained by allowing the light from a source of negligible extension to pass through a very small opening in an opaque screen. The light which reaches the space behind the screen will fill a region the boundary of which (the edge of the pencil) will, at first sight, appear to be sharp. A more careful examination will reveal, however, that the light intensity near the boundary varies rapidly but continuously from darkness in the shadow to lightness in the illuminated region, and that the variation is not monotonic but is of an oscillatory character, manifested by the appearance of bright and dark bands, called diffraction fringes. The region in which this rapid variation takes place is only of the order of magnitude of the wavelength. Hence, as long as this magnitude is neglected in comparison with the dimensions of the opening, we may speak of a sharply bounded pencil of rays.[†] On reducing the size of the opening down to the dimensions of the

⁴ That the boundary becomes sharp in the limit as λ₀ → 0 was first shown by G. Kirchhoff, *lorlerungen û. Math. Phys.*, Vol. 2 (*Mathematische Optik*) (Leipzig, Tuebner, 1891), p. 33. See also B. B. Baker and E. T. Copson, *The Mathematical Theory of Haygens' Principle* (Oxford, Clarendon Press, 2nd edition, 1950), p. 39, and A. Sommerfeld, *Optics* (New York, Academic Press, 1954), §35.

116

⁸ The historical development of geometrical optics is described by M. Herzberger, Struklenoptik (Berlin, Springer, 1931), p. 179; Z. Instrumentenkunde, 52 (1932), 429–435, 485–493, 534–542, C. Carathéodory, Geometrische Optik (Berlin, Springer, 1937) and E. Mash, The Principles of Physical Optics, A Historical and Philosophical Treatment (First German edition 1913), English translation: London, Methuen, 1926; reprinted by Dworr Publications, New York, 1953).

Geometrical Optics of Electromagnetic Fields

 $\frac{3.1 \text{ Approximation for very short wavelengths}}{\text{But by (38), (15) and (25),}}$ $d\tau = \frac{dS}{(\operatorname{crad} S)^2} = \frac{1}{n^2} dS = \frac{1}{n} ds, \qquad (39)$

so that we finally obtain the following expressions for the ratio of the intensities at any two points of a ray:

$$\frac{I_2}{I_1} = \frac{n_2}{n_1} e^{-\int_{S_1}^{S_2} \frac{y^2 g}{s^2} dS} = \frac{n_2}{n_1} e^{-\int_{S_1}^{S_2} \frac{y^2 g}{s} ds},$$

(40)

the integrals being taken along the ray.*

3.1.3 Propagation of the amplitude vectors

We have seen that, when the wavelength is sufficiently small, the transport of energy may be represented by means of a simple hydrodynamical model which may be completely described in terms of the real scalar function S, this function being a solution of the eikonal equation (15). According to traditional terminology, one understands by geometrical optics this approximate picture of energy propagation, using the concept of rays and wave-fronts. In other words polarization properties are excluded. The reason for this restriction is undoubtedly due to the fact that the simple laws of geometrical optics concerning rays and wave-fronts were known from experiments long before the electromagnetic theory of light was established. It is, however, possible, and from our point of view quite natural, to extend the meaning of geometrical optics to embrace also certain geometrical laws relating to the propagation of the "amplitude vectors" e and h. These laws may be easily deduced from the wave equations (16)–(17).

Since S satisfies the eikonal equation, it follows that $\mathbf{K} = 0$, and we see that when k_0 is sufficiently large (λ_0 small enough), only the *L*-terms need to be retained in (16) and (17). Hence, in the present approximation, the amplitude vectors and the eikonal are connected by the relations $\mathbf{L} = 0$. If we use again the operator $\partial/\partial \tau$ introduced by (38), the equations $\mathbf{L} = 0$ become

$$\frac{\partial \mathbf{e}}{\partial \tau} + \frac{1}{2} \left(\nabla^2 S - \frac{\partial \ln \mu}{\partial \tau} \right) \mathbf{e} + (\mathbf{e} \cdot \operatorname{grad} \ln n) \operatorname{grad} S = 0, \quad (41)$$

$$\frac{\partial \mathbf{h}}{\partial \tau} + \frac{1}{2} \left(\nabla^2 S - \frac{\partial \ln \varepsilon}{\partial \tau} \right) \mathbf{h} + (\mathbf{h} \cdot \operatorname{grad} \ln n) \operatorname{grad} S = 0. \quad (42)$$

These are the required *transport equations* for the variation of e and h along each ray. The implications of these equations can best be understood by examining separately the variation of the magnitude and of the direction of these vectors.

* It has been shown by M. Kline, Comm. Pure and Appl. Mathx., 14 (1961), 473 that the intensity ratio (40) may be expressed in items of an integral which involves the principal ndii of curvature of the associated wavefoots. Kline's formula is a natural generalization, to inhomogeneous media, of the formula (34). See also M. Kline all. W. Kay, it'di, 184.

page 125

"According to traditional terminology, one understands by geometrical optics this approximate picture of energy propagation, using the concept of rays wave-fronts. In other and words polarization properties are excluded. The reason for this restriction is undoubtedly due to the fact that the simple laws of geometrical optics concerning rays and wave-fronts were known from experiments long before the electromagnetic theory of light was established. It is, however, possible, and from our point of view quite natural, to extend the meaning of geometrical optics to embrace also certain geometrical laws relating to the propagation of the 'amplitude vectors' E and H."

We follow Max Born's and Emil Wolf's point of view!



Development and implementation of algorithms to solve Maxwell's equations in its **geometric field approximation**!



Source and System Modeling



Source and System Modeling



System Modeling Example

Provided by Idir Mourad, BNL







Measured error map, PV ~ 1.2 nm provided by Idir Mourad, BNL



Image: Start Sources Functions Catalogs Windows Light Path	Wyrowski VirtualLab Fusion (User Experience Edition (Build 6.2.1.15)) — 🗇 🗙
Gol Simulation Parameter Security Parameters New You finize Detector Positions Use F Execution Parameters Parameter Run M Find Focus Position Co	arameter Edit Parameter pling Coupling Vew Smullation View Vew	
Interfaces Catalog Definition Type Light Trans Defined	Edit Sinole Onticel Interface X	Combined Interface X ture Height Discontinuities Scaling Coating Periodization rface Definitions Interface 2 ampled Interface Programmable Interface Inition Area Interface 2 ace and Shape Rectangular Shape Rectangular O Field Passes Plane Interface Interface Interface Interface Image: Coating Plane Specification Mode Image: Coating Plane Specification Mode Image: Coating Plane Isolation Fined Image: Coating Plane Specification Mode Image: Coating Plane Isolation Fined Image: Coating Plane Isolation Image: Coating Plane Specification Mode Image: Coating Plane Isolation Image: Coating Plane Isolation Image: Coating Isolation Image: Coating Plane Isolation Image: Coating Plane <t< th=""></t<>
Detector Results Date/Time Detector	Sub-Detector	Result



Date/Time	Detector	Sub - Detector	Result				
Detector Results						Ф	
	Image: Simulation Engine Geometric Field Tracing Plus (Beta) ✓						
		le					
Check Cons	stency validity: 🗸	UK Cancel Help	OK Cancel Help				
٢		>		_			
40 return	height;		s 🖓 🚽 Validity: 🗸 🛛 OK Cancel H	elp			
39	holekt.						
38 beight = -1 * (-(xx - x0) * sin + (zp - z0) * cos); /* multiply with -1 as it turns the h 0 0 2.Position							
36 Complex Root2 = Math.Sqrt(1 - xx * xx / (a * a)); double zra = b * Root2 Re + ze:							
35 double	35 double xx = (-q + Rootl.Re) / (2 * p); /* The start and ending point before rotating it						
34 Complex	<pre>k Root1 = Math.Sqrt(q * q - 4 * p * r1);</pre>	1 T Z (A T ZO SIII) AO	n Mode				
32 double	$q = -2 * x0 * \cos * \cos - 2 * (x + z0 * \sin) * \cos;$ $r1 = (x + z0 * \sin) * (x + z0 * \sin) - h * h * \sin * \sin $	n + 2 * (x + 70 * sin) * x0	Def. Area				
31 double	p = b * b * sin * sin / (a * a) + cos * cos;						
29 sin = 1 30 cos = 1	Math.Cos(Phi2);/**/	psorbed					
28 double	Phi2 = Math.Atan(-b * b / (a * a) * x0 / z0); /* Angle	between x-axis and slope of	ses Plane Interface				
27	all constants are fixed and ellipse is well defined, no	w carculace the million in c	Dutside of Definition Area				
25 26 /* Now	all constants are fixed and ellinse is well defined No	w calculate the mirror in t					
24 double	z0 = -b / (4 * Fx * a) * z0root.Re;		200 mm				
23 Complex	<pre>x z0root = Math.Sqrt(16 * Fx * Fx * a * a - DeltaF * Del</pre>	taF);	Rectangular O Elliptic				
21 double	<pre>b = broot.Re;/* This is the size of the parabola in the x0 = DeltaF / (4 * Fx): /* location where ray bits under</pre>	height direction */		_			
20 Complex	<pre>k broot = Math.Sqrt(a * a - Fx * Fx);</pre>			_			
19 double	<pre>Fx = FxC.Re; /* should be real always and smaller then</pre>	a*/					
17 double	<pre>Fx2 = 16 * a * a * (DeltaF / (4 * a * a) + 1) * (DeltaF</pre>	/ (4 * a * a) + 1);				rer	
The double	Fx1 = F1 * F1 * DeltaF * DeltaF * cos * cos / (a * a) -	DeltaF * DeltaF * (DeltaF	✓ Edit Manue Calibraty / Edit Manue			2 plos	
8 15 /* 2*F	<pre>v = distance between (point) source and focus */</pre>	F2 [double]	ace Programmable Interface			abE	
🔮 13 double	<pre>a = (F1 + F2) / 2; /* size of parabola in x-direction * Doltar</pre>	/ Angle [double] F1 [double]				ualL	
ੱੂ 12 double	<pre>sin = Math.Sin(Ang);</pre>	y [double]	Interface 2			Virt	
E 11 double	<pre>cos = Math.Cos(Ang);</pre>	Aperture Diameter Y [double]	a) ons			4	
5 10		Aperture DiameterX [double	Discontinuities Scaling Coating Periodization			owse	
Source Code Global Paran	neters Advanced Settings		terface	×		y Bro	
Source Code Editor			×	×		opert	
						^ P	
Execution Parameters	Parameter Variation	View					
+ Settings Overview	w Parameter Run 🐝 Find Focus Position Coupling Coupling	System Report					
Go! Simulation Parameter	er New Optimize Detector Positions Use Parameter Edit Parameter	View Simulation					
🕨 🦾 🗊	New Parametric Optimization	30					
Start Sources	Functions Catalogs Windows Light Path Tools						
	Light Path	wyrowski virtuaicab Fusion (User Ex	penence Edition [Build 0.2.1.13])		ð	×	
📕 🖓 🖬 😂 🗔 🕮 💷	THE REPORT OF	Wyrawski Virtuall ab Eurion /Urar Ev	mariance Edition (Puild 6.2.1.151)		1 march	100	

Image: Start Sources Functions Catalogs Windows Light I	ight Path V Path Tools	Wyrowski VirtualLab Fusion (User Experience Edition [Build 6.2.1.15])	-	٥	× @•
Go! Simulation Parameter Settings Overview Execution Parameters Parameter Run % Find Focus Position Parameter Variat	n System Report Coupling View				
Compared Break Components Control tele Break Components Control tele Break Components Detectors A rayzers Control tele Break Components Detectors Control tele Break Components Control tele Break Components Detectors Control tele Break Components Detectors Control tele Break Components Setter Tele Control tele Contro	20160728_Elliptical/Mirrors_Case3.lpd =1)* C C C C C C C C C C C C C C C C C C C	Edit Single Optical Interface Edit Combined Interface Structure Height Discontinuities Scaling Coating Interface Definitions Interface Definitions Interface 1 Sampled Interface Interface 1 Interface 1 Sampled Interface Interface 1 Interface	Periodization Interface 2 Programmable Interface Load Edit View OElliptic 12mm OK Cancel Help OK Cancel Help OK Cancel Help Gt		Property Browser VirtualLab Explorer
Date/Time Detect	r Sub	- Detector	Result		



Case	Strehl Ratio	
Ideal	1.0000	
1x Errormap	0.9933	
5x	0.9445	
10x	0.7903	
20x	0.3964	

Measured error map, PV ~ 1.2 nm provided by Idir Mourad, BNL





VirtualLab Fusion is a fast physical optics modeling and design software.

Could be powerful tool for x-ray modeling!





We encourage you to contact us to find out, how good we can treat with your modeling and design tasks.

Common paper as result would be fine!