

Refractive indices for extraordinary waves in uniaxial crystals

Zhongxing Shao

*Changchun Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, P.O. Box 1024,
Changchun 130022, People's Republic of China*

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In order to support our earlier experimental investigation of extraordinary rays' behavior in uniaxial crystals [Zhongxing Shao and Chen Yi, *Appl. Opt.* **33**, 1209 (1994)], as well as to determine the indices of refraction for the extraordinary waves at arbitrary incidence and in arbitrary orientation of the optical axis, and to compare with our experimental results, the ellipsoidal equation depicting double refraction propagation is solved with the expressions given in terms of the easily measured parameters: incident angle θ , rotational angle Φ of the crystal, and the inclined angle η of the axes. Based on the solutions, the refractive angle r_p of the ray (or the Poynting vector) and the angle β_p between the ray and the optical axis, as well as the refractive angle r_w of the wave normal of the extraordinary wave and the angle β_w between the normal and the axis are given. The results of the indices of refraction for the extraordinary waves are practically presented by applying the derived angles combined with the equation [A. Yariv, *Quantum Electronics*, 2nd ed. (Wiley, New York, 1975)]:

$$1/n_e^2(\beta_w) = \cos^2(\beta_w)/n_o^2 + \sin^2(\beta_w)/n_e^2.$$

As an example of application, the indices of calcite and quartz are calculated using some angular parameters. To clarify the divergence [M. Born and E. Wolf, *Principles of Optics*, 5th ed. (Pergamon, New York, 1975); F. A. Jenkins and H. E. White, *Fundamentals of Optics*, 4th ed. (McGraw-Hill, New York, 1976), p. 508], regarding the index and by analogy with Snell's law, the ratio $n_e(r_w) = \sin(\theta)/\sin(r_w)$ is also discussed.

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I. INTRODUCTION

The extraordinary rays in double refraction crystals are a long-recognized optical phenomenon. Almost all optical textbooks have mentioned it, and some recent articles have discussed the tracing of the ray [1-7] as well, but as far as we know, it has not been described satisfactorily. Consequently, the indices of refraction for the extraordinary waves have not yet been established unequivocally. Although we have had the familiar formula

$$1/n_e^2(\beta_w) = \cos^2(\beta_w)/n_o^2 + \sin^2(\beta_w)/n_e^2 \quad (1)$$

to calculate theoretically the index $n_e(\beta_w)$, where n_o and n_e are the principal indices of the ordinary and the extraordinary waves, respectively, the problem is how to practically define the angle β_w between the wave normal of the extraordinary wave and the optical axis with measurable quantities. The expression

$$\cos\beta_w = \cos\Phi \cos\theta \quad (2)$$

has been frequently used [8], where Φ is the rotation angle of the optical axis (or the crystal) away from the incident plane (while $\Phi=0$, the axis is in the plane). Unfortunately, Eq. (2) is valid only for crystals with optical axes parallel to the surface (CAPS). Even then, it is constrained by the limitations of incidence at the Brewster angle and the wave normal must be assumed to stay in the incident plane, whatever Φ is. In addition, the ambi-

guous expression, $\sin(\theta)/\sin(r_w) = n_e$, where r_w is the refractive angle of the wave normal, was employed in the derivation of Eq. (2). As we pointed out in Ref. [1] the wave normal does not stay in the plane unless the axis is in the plane; the expression is not correct except when the axis is vertical to the plane. Equation (1) is nevertheless very useful in some theoretical analyses in crystal and nonlinear optics for assigning a preliminary angle β_w .

Our earlier experimental studies on the extraordinary rays' behavior [1] revealed the following. (i) While the crystal with optical axes inclined to the surfaces (CAIS) is turned around the normal, the ray always rotates around the ordinary ray. When the crystal is turned to π , the ray rotates to π . But the rotation is not in step with the turning. For the CAPS the ray rotates up to π while the crystal is only twisted to $\pi/2$. (ii) The traces of the ray on the emerging surface in the CAIS, surprisingly, are a series of curves that resemble the Pascal worms at different incident angles. In CAPS, the traces degenerate to a series of ellipses. (iii) For CAPS, Snell's law is tenable only in the case where the axes are perpendicular to the incident plane.

Based on these discoveries, we have solved the ellipsoidal equation depicting the ray's propagation and determined three-dimensional coordinates that prove useful for tracing the extraordinary ray. Then the refractive angle of the ray (which is specifically the angle between the ray and the normal of the crystal and the angle between the ray and the optical axis), the refractive angle of the

wave normal, and the angle between the wave normal and the axis are obtained in terms of the easily measurable angular parameters θ , Φ , and η . Fitting the angle between the wave normal and axis to Eq. (1), the indices for the extraordinary waves can be determined in practical experiments.

II. THE COORDINATES OF THE EXTRAORDINARY RAY

A movable rectangular system $OX'Y'Z'$ is chosen to aid in the analysis of a uniaxial crystal in arbitrary orientation of the optical axis. The OY' axis is in the same direction as the axis OA (see Fig. 1). The ellipsoidal equation in the system can be written as

$$n_e^2 X'^2 + n_o^2 Y'^2 + n_e^2 Z'^2 = 1. \quad (3)$$

After rotating the $OX'Y'Z'$ system in such a way that the OY' axis is first turned at an angle η around the OX' axis, then at angle Φ around the OZ' axis, the system $OXYZ$ is set in the same way as the original orientation of the $OX'Y'Z'$ used to observe the rays' behavior. The OXY plane is on the front surface and the OZ axis coincides with the normal of the crystal. Equation (3) can be rewritten, in the system being observed, as

$$F_x X^2 + F_y Y^2 + BZ^2 + F_{xy}XY + F_{yz}YZ + F_{zx}ZX = 1, \quad (4)$$

with

$$\begin{aligned} F_x &= n_e^2 \cos^2 \Phi + A \sin^2 \Phi, \\ F_y &= n_e^2 \sin^2 \Phi + A \cos^2 \Phi, \\ A &= n_o^2 \cos^2 \eta + n_e^2 \sin^2 \eta, \\ B &= n_o^2 \sin^2 \eta + n_e^2 \cos^2 \eta, \\ F_{xy} &= (n_e^2 - n_o^2) \sin(2\Phi) \cos^2 \eta, \\ F_{yz} &= (n_e^2 - n_o^2) \cos \Phi \sin(2\eta), \\ F_{zx} &= (n_o^2 - n_e^2) \sin \Phi \sin(2\eta). \end{aligned}$$

All the factors in Eq. (4) are in terms of the angular parameters η and Φ only. But, generally, η is fixed once the crystals are cut for use as an optical component. Hence, our interest in the index for the extraordinary wave focuses on its relation to Φ in the foregoing analysis.

A beam making an arbitrary angle θ is incident on the crystal. It is divided into the ordinary and the extraordinary rays, OE_o and OE_e , respectively, as it enters the crystal. The point $P(X_1, Y_1, Z_1)$ observed on the extraordinary ray satisfies Eq. (4),

$$F_x X_1^2 + F_y Y_1^2 + BZ_1^2 + F_{xy} X_1 Y_1 + F_{yz} Y_1 Z_1 + F_{zx} Z_1 X_1 = 1. \quad (5)$$

On the other hand, when considering point P' to be of equal optical path to P , we find that the distance from O to P' $d(OP') = ct/\sin\theta$. For the sake of convenience, taking the time $t = 1/c$ [c denotes the light velocity; actually, it is under this assumption that Eq. (3) is obtained. Note that the incident plane is the OYZ plane (refer to

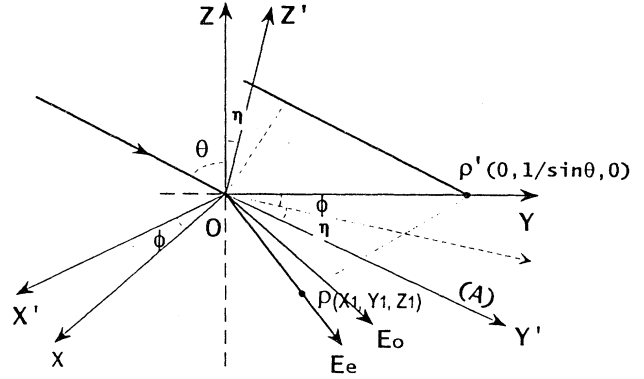


FIG. 1. A movable rectangular system $OX'Y'Z'$ is rotated in such a way that the OY' axis is turned an angle η around the OX' axis first, then angle Φ around the OZ' axis. The stationary system $OXYZ$ is set as the original orientation, as the $OX'Y'Z'$ system used to be for observing the extraordinary ray's behavior. P' is the point where the optic path is equal to the point P being observed. $d(OP') = ct/\sin\theta$ (t denotes the time, c the light velocity).

Fig. 1 or 2)], the coordinates of P' should be $(0, 1/\sin\theta, 0)$. Hence, the tangent equation going through points P and P' is found to be

$$F_y Y_1 + F_{xy} X_1 / 2 - F_{yz} Z_1 / 2 = \sin\theta$$

or

$$Y_1 = (2 \sin\theta - F_{xy} X_1 + F_{yz} Z_1) / (2 F_y). \quad (6)$$

Substituting Eq. (6) into (5), we have

$$X_1 = (b \pm \sqrt{b^2 - 4ac}) / (2a), \quad (7)$$

where

$$\begin{aligned} b &= [F_{zx} - F_{xy} F_{yz} / (2 F_y)] Z_1, \\ a &= F_x - F_{xy}^2 / (4 F_y), \\ c &= [B - F_{yz}^2 / (4 F_y)] Z_1^2 + \sin^2(\theta) / F_y - 1. \end{aligned}$$

In order to find Z_1 , X_1 in Eq. (5) must be zero. (Making Z_1 equal to zero apparently does not make sense, because it means the light would not have entered the crystal. Alternatively, if $Y_1 = 0$, it would confine the case to normal incidence.) Then Eqs. (5) and (6) simplify to

$$F_y Y_1^2 + BZ_1^2 + F_{yz} Y_1 Z_1 = 1 \quad (8)$$

or

$$\begin{aligned} [Z_1 + F_{yz} Y_1 / (2B)]^2 / (1/\sqrt{B})^2 \\ + Y_1^2 / [1/\sqrt{F_y} - F_{yz}^2 / (4B)]^2 = 1 \end{aligned}$$

and

$$Y_1 = (2 \sin\theta - F_{yz} Z_1) / (2 F_y). \quad (9)$$

Evidently, Eq. (8) is an ellipselike equation describing the intersecting curve between the ellipsoid and the OYZ

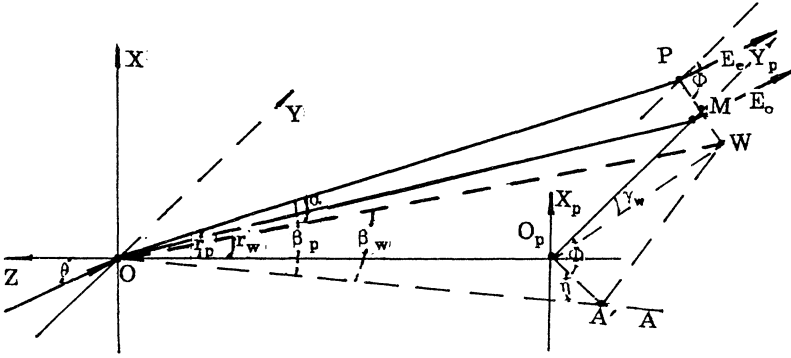


FIG. 2. Diagram showing the rotation of the extraordinary ray (the Poynting vector) around the ordinary ray and the wave normal of the extraordinary wave around the extraordinary ray while the optical axis is rotated at an angle Φ . OP denotes the Poynting vector. OW , which is separated by a small angle α from OP , represents the wave normal. The coordinates of point P are (X_1, Y_1, Z_1) . β_p is the angle between the extraordinary ray and the axis. β_w indicates the angle between the wave normal and the axis. r_p and r_w are the refractive angle of the ray and the wave normal, respectively.

plane. One of its axes $1/\sqrt{B}$, does not relate to Φ , but the other one does. Anyway, substituting Eq. (9) into (8), we obtained

$$Z_1^2 = 4(F_y - \sin^2\theta)/(4BF_y - F_{yz}^2). \quad (10)$$

Taking into account Eq. (10), Z_1^2 should attain one of its extreme values, as F_{yz} becomes maximum at $\Phi=0$:

$$Z_0^2 = (A - \sin^2\theta)/(n_0^2 n_e^2).$$

On the other hand, if F_{yz}^2 becomes zero at $\Phi=\pi/2$, then Z_1^2 should change to another extreme value,

$$Z_{\pi/2}^2 = A(n_e^2 - \sin^2\theta)/(n_0^2 n_e^4).$$

The two extreme values of Z_1^2 are only related to the angular variables θ and η .

Next we are going to determine the varying rule of Z_1 for changing Φ . To accomplish this, it is important to note the factor F_y with regard to the Y axis (so that it relates to the optical axis), which aids in coordinate transfer. The fact can be rewritten as

$$F_y = A - (A - n_e^2)\sin^2\Phi. \quad (11)$$

For simplicity, by making $\eta=0$ (which leads to $A=n_0^2$), Eq. (11) is simplified to

$$F_y = n_0^2 - (n_0^2 - n_e^2)\sin^2\Phi. \quad (11')$$

If the coordinate axes, X, Y, Z , are changed to the principal indices, i.e., $Y=n_0, X=Z=n_e$, then the ellipsoidal equation can be regarded as the index ellipsoid. So, Eq. (11') proves that the indices in the CAPS, owing to the change of Φ , vary from the ordinary ray's principal index (when $\Phi=0$) to that of the extraordinary wave (when $\Phi=\pi/2$). The rule for varying between the two extreme values (the principal indices) follows the sinusoidal ($\sin^2\Phi$) pattern. The increment of the variation is $(n_0^2 - n_e^2)\sin^2\Phi$. Comparing Eqs. (11) and (11'), we see that the variation rule for the CAIS is the same as that for CAPS, except that the term A should be replaced with n_0^2 . Returning to the matter of rays propagation, similarly to the index, Z_1^2 varies between the two extreme values (Z_0^2 and $Z_{\pi/2}^2$):

$$Z_1^2 = Z_0^2 - (Z_0^2 - Z_{\pi/2}^2)\sin^2\Phi.$$

This means that while the optical axis is in the incident

plane, Z_1^2 becomes Z_0^2 and the observation point P is in the plane OXZ ($X=0$). Once the axis is rotated away from the plane, Z_1^2 will decrease by the increment $(Z_0^2 - Z_{\pi/2}^2)\sin^2\Phi$. When the axis is again perpendicular to the plane, Z_1^2 will attain the other extreme $Z_{\pi/2}^2$. At the same time, X_1 no longer equals zero until the axis returns to the plane. Point P will travel around the rim of the ellipsoid.

So far, all three coordinates needed to describe the extraordinary ray's behavior are solved in terms of the easily measured angular parameters θ, Φ, η and the known principal indices n_0 and n_e .

III. THE ANGLES $r_p, \beta_p, r_w, \beta_w$ AND THE INDICES

Having found the coordinates describing the extraordinary rays, the refractive angle of the extraordinary ray, r_p , and the angle between the ray and the optical axis, β_p , as well as the refractive angle of the wave normal, r_w , and the angle between the normal and the axis, β_w , can be defined with the coordinates and the angles θ, Φ, η .

When $\Phi=0$, we know that the optical axis, the extraordinary ray, and the wave normal to the extraordinary wave are coplanar and in the incident (OXY) plane. Note that the wave normal should lie to the right of the extraordinary ray in order to conform to the indices of refraction: at any incidence and in any orientation of the optical axis, they are confined within the principal indices n_0 and n_e .

When the optical axis OA rotates at an angle Φ around the OZ axis away from the OYZ plane, the extraordinary ray rotates to OP . To keep the ray, the wave normal, the electrical vector, and the displacement vector coplanar as well as perpendicular to the magnetic vector (or the magnetic induction), according to Refs. [4] and [9], the wave normal OW must rotate around the ray in the same direction as OA 's rotation and at the same angle as Φ to follow the rotation of the electrical vector of the ray (see Fig. 2). Generally, the wave normal is separated a small angle (several degrees) α from the ray. Because of the double refraction angle α , the extraordinary wave normal is confined to a single side (which side depends on whether the crystal is positive or negative) as compared to the ordinary ray (wave), although the extraordinary ray rotates around the ordinary ray while the crystal is being turned. The angle α , according to Ref. [10], equals

$$\tan\alpha = (n_0^2/2)(1/n_e^2 - 1/n_0^2)\sin(2\beta_w) .$$

Taking into account the coordinate plane of point P , $O_P X_P Y_P$, which is parallel to and has a separate Z_1 from the OXY plane, we can easily determine the refractive angle of the extraordinary ray and the extraordinary wave normal, respectively,

$$\cos(r_p) = Z_1/d(OP) , \quad (12)$$

with

$$[d(OP)]^2 = X_1^2 + Y_1^2 + Z_1^2 ,$$

and

$$\cos(r_w) = Z_1/d(OW) , \quad (13)$$

with

$$OW = (X_w^2 + Y_w^2 + Z_w^2)^{1/2} ,$$

where X_w, Y_w, Z_w are the coordinates of the point W and

$$\begin{aligned} X_w &= X_1 - d(PW)\sin\Phi , \\ Y_w &= Y_1 + d(PW)\cos\Phi , \\ Z_w &= Z_1 . \end{aligned} \quad (14)$$

$d(PW)$ in Eqs. (14) is a function of α and is solved in the Appendix. (Note that $d(OW)$ should be shorter than $d(OP)$ because the phase velocity is the projection of the ray velocity on the direction of the wave normal, so that point W should not be in the $O_P X_P Y_P$ plane. Here, for convenience, we extend the normal so that it intersects the plane, since the extension does not affect the angles.

Considering triangle OPA' (the plane $O_P X_P Y_P$ intersects the optical axis at point A'), we find the angle β_p :

$$\cos\beta_p = [d^2(OP) + d^2(OA') - d^2(PA')]/2d(OP)d(OA') . \quad (15)$$

Applying the coordinates of point P and Eq. (12), and with proper mathematical operations, Eq. (15) can be rewritten as

$$\cos\beta_p = \sin(r_p)\cos\eta\cos(\Phi + \gamma_p) + \cos(r_p)\sin\eta , \quad (16)$$

with

$$\tan(\gamma_p) = X_1/Y_1 .$$

In the same way, the angle between the wave normal and the axis, β_w , can be determined in triangle $OA'W$:

$$\cos\beta_w = [d^2(OW) + d^2(OA') - d^2(A'W)]/2d(OW)d(OA') . \quad (17)$$

All the terms on the right-hand of Eq. (17) are solved in the Appendix. With the help of Eqs. (13) and (14), we can also write Eq. (17) in the form of angular variables:

$$\cos\beta_w = \sin(r_w)\cos\eta\cos(\Phi + \gamma_w) + \cos(r_w)\sin\eta , \quad (18)$$

with

$$\tan(\gamma_w) = X_w/Y_w .$$

Equations (16) and (18) do not have the problems incurred in Eq. (2) because they do not use the ambiguous expression $\sin(\theta)/\sin(r_w) = n_e$ and also because of the assumption that the wave normal must be in the incident plane no matter what the positions of the optical axis is. Hence, they are more general than Eq. (2). In fact, Eqs. (16) and (18) could be simplified to Eq. (2) if the axis were parallel to the surface and perpendicular to the incident plane, $\gamma = X_1/Y_1 = 0$ ($X_1 = 0$ in this case), so that $\gamma' = 0$. And note that if θ is the Brewster angle, $\sin(r_p)$ or $\sin(r_w)$ can be replaced with $\cos\theta$ by using the ambiguous expression $\sin(\theta)/\sin(r_w) = n_e$.

Substituting Eq. (18), at last, into Eq. (1), the indices for the extraordinary wave can be determined at any incidence and in arbitrary orientation of the optical axis.

As concrete examples of applying the angle β_w , the indices of calcite and quartz are calculated and listed in Table I. The parameters used in the calculations are $\eta = 45.93^\circ$ for calcite (natural cleavage), 45° for quartz, and $n_0 = 1.65836$, $n_e = 1.48641$ for calcite, $n_0 = 1.54425$, $n_e = 1.55336$ for quartz. For the sake of showing the agreement between the equations derived here and the ex-

TABLE I. The indices of refraction for the extraordinary waves, $n_e(\beta_w)$ for calcite and quartz, and the sine ratio $n_e(r_w)$ for calcite only. The parameters applied in the calculations are $\eta = 45.93^\circ$ for calcite (natural cleavage) and 45° for quartz. The principal indices $n_0 = 1.65836$, $n_e = 1.48641$ for calcite, $n_0 = 1.54425$, $n_e = 1.55336$ for quartz.

Φ	$n_e(\beta_w)$				$n_e(r_w)$			
	$\theta = -\pi/6$		$\theta = \pi/4$		$\theta = \pi/3$		$\theta = 5\pi/12$	
	calcite	quartz	calcite	quartz	calcite	quartz	calcite	quartz
0	1.62099	1.54594	1.63847	1.54506	1.64913	1.54456	1.65412	1.54435
$\pi/8$	1.61552	1.54624	1.62986	1.54549	1.63766	1.54510	1.64054	1.54496
$\pi/5$	1.56238	1.54713	1.57248	1.54672	1.60873	1.54659	1.60749	1.54655
$3\pi/8$	1.58090	1.54823	1.57852	1.54818	1.57340	1.54839	1.56852	1.54860
$\pi/2$	1.56031	1.54925	1.55043	1.54972	1.54067	1.55019	1.53361	1.55054
$5\pi/8$	1.53923	1.55023	1.52379	1.55099	1.51182	1.55160	1.50460	1.55199
$3\pi/8$	1.52642	1.55095	1.50916	1.55185	1.49784	1.55247	1.49218	1.55281
$7\pi/8$	1.52065	1.55137	1.50319	1.55231	1.49291	1.55289	1.48858	1.55315
π	1.51913	1.55150	1.50171	1.55245	1.49180	1.55300	1.48790	1.55324

TABLE II. Comparison between calculation and experiment of the refractive angles (in degrees) of the extraordinary ray, r_p , in calcite.

Φ	$\theta = \pi/6$		$\theta = \pi/4$		$\theta = \pi/3$		$\theta = 5\pi/12$	
	calc.	expt.	calc.	expt.	calc.	expt.	calc.	expt.
0	12.70	13.01	21.46	21.42	28.77	28.60	33.73	33.78
$\pi/8$	13.83	13.23	22.59	23.03	29.93	29.77	34.90	35.33
$\pi/4$	16.43	14.35	25.23	26.15	32.62	32.84	37.63	38.17
$3\pi/8$	19.21	17.03	28.05	28.21	35.44	35.85	40.43	40.77
$\pi/2$	21.42	19.49	30.15	30.05	37.39	37.66	42.26	42.22
$5\pi/8$	23.13	23.00	31.60	31.04	38.37	38.37	42.84	42.53
$8\pi/4$	23.83	23.65	31.78	31.22	38.25	38.56	42.49	42.01
$7\pi/8$	23.96	23.97	31.59	31.14	37.76	37.96	41.86	41.72
π	23.94	24.12	31.46	31.26	37.52	37.49	41.55	41.50

periments in Ref. [1], the refractive angles of the ray for calcite are listed in Table II.

IV. CONCLUSION AND DISCUSSION

The ellipsoidal equation depicting double refraction propagation is solved by setting up the coordinate equations describing the extraordinary ray's behavior with the easily measured angular parameters. Based on the solutions, the equations with respect to the refractive angle of the ray, r_p , and the angle β_p between the ray (or the Poynting vector) and the optical axis, as well as the refractive angle r_w and the angle β_w between the axis and the wave normal of the extraordinary wave, are given. They are applicable to CAIS [of course, to CAPS as well, provided the inclined angle of the axis η in Eq. (18) equals zero] at any incidence and for arbitrary rotation of the crystal. By applying these solutions together with Eq. (1), it is now feasible to determine the indices of refraction for the extraordinary wave with experimentally measurable parameters. As an example of application, we calculated the indices for calcite and quartz under some angular parameters and listed than in Table I.

By analogy with Snell's law for the extraordinary wave, we have

$$\sin(\theta)/\sin(r_w) = n_e(r_w).$$

To identify the sine ratio from the index, $n_e(r_w)$ for calcite at $\theta = \pi/3$ is also listed in Table I. Apparently, the ratio does not equal $n_e(\beta_w)$. Also, we calculated the ratio $\sin(\theta)/\sin(r_p)$ for the extraordinary ray, which also does not equal the index. Therefore, Snell's law is generally not valid for either the extraordinary wave or the extraordinary ray, except when the axis is both parallel to the surface and perpendicular to the incident plane.

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APPENDIX

To work out the coordinates of $W(X_w, Y_w, Z_w)$, which define the point of intersection between the extended extraordinary wave normal and the coordinate surface of point P (see Fig. 2),

$$X_w = X_1 - d(PW) \sin \Phi,$$

$$Y_w = Y_1 + d(PW) \cos \Phi,$$

$$Z_w = Z_1,$$

the segment PW should be settled as

$$d(PW) = d(OP) \sin(\alpha) / \sin(\alpha + \angle OPW),$$

with

$$d^2(OP) = X_1^2 + Y_1^2 + Z_1^2,$$

$$\cos(\angle OPW)$$

$$= [d^2(OP) + d^2(PM) - d^2(OM)] / 2d(OP)d(PM)$$

and

$$d(PM) = X_1 / \sin \Phi,$$

$$d^2(OM) = Z_1^2 + d^2(O_P M),$$

$$d(O_P M) = Y_1 + X_1 / \tan \Phi.$$

To work out β_w with an expression of angular variables as

$$\cos \beta_w = \sin(r_w) \cos \eta \cos(\Phi + \gamma_w) + \cos(r_w) \sin \eta,$$

the following equations are necessary:

$$\cos \beta_w = [d^2(OW) + d^2(OA') - d^2(A'W)] / 2d(OW)d(OA'),$$

with

$$d(OW) = Z_1 / \cos(r_w),$$

$$d(OA') = Z_1 / \sin \eta,$$

$$d^2(A'W) = [d^2(O_P W) + d^2(O_P A') - 2d(O_P W)d(O_P A') / \cos(\Phi + \gamma')],$$

and

$$d(O_P W) = Z_1 x \tan(r_w),$$

$$d(O_P A') = Z_1 / \tan \eta.$$

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