International Tables for Crystallography (2013). Vol. D, Table 1.7.2.3, p. 186.

lographical frame by the standard conventions given in Chapter 1.6.

1.7.3. Propagation phenomena

1.7.3.1. *Crystalline linear optical properties*

We summarize here the main linear optical properties that govern the nonlinear propagation phenomena. The reader may refer to Chapter 1.6 for the basic equations.

1.7.3.1.1. *Index surface and electric field vectors*

The relations between the different field vectors relative to a propagating electromagnetic wave are obtained from the constitutive relations of the medium and from Maxwell equations.

In the case of a non-magnetic and non-conducting medium, Maxwell equations lead to the following wave propagation equation for the Fourier component at the circular frequency ω defined by (1.7.2.15) and (1.7.2.16) (Butcher & Cotter, 1990):

$$\nabla \mathbf{x} \nabla \mathbf{x} \mathbf{E}(\omega) = (\omega^2/c^2)\mathbf{E}(\omega) + \omega^2 \mu_0 \mathbf{P}(\omega), \qquad (1.7.3.1)$$

where $\omega = 2\pi c/\lambda$, λ is the wavelength and c is the velocity of light in a vacuum; μ_0 is the free-space permeability, $\mathbf{E}(\omega)$ is the electric field vector and $\mathbf{P}(\omega)$ is the polarization vector.

Table 1.7.2.3. *Nonzero $\chi^{(2)}$ coefficients and equalities between them under the Kleinman symmetry assumption*

Symmetry class	Independent nonzero $\chi^{(2)}$ elements under Kleinman symmetry
Triclinic	
C_1 (1)	xxx, $xyy = yxy = yyx$, $xzz = zxz = zzx$, $xyz = xzy = yxz = yzx = zxy = zyx$, $xxz = xzx = zxx$, $xxy = xyx = yxx$, yyy, $yzz = zyz = zzy$, $yyz = yzy = zyy$, zzz
Monoclinic	
C_2 (2) (twofold axis parallel to z)	$xyz = xzy = yxz = yzx = zxy = zyx$, $xxz = xzx = zxx$, $yyz = yzy = zyy$, zzz
C_s (m) (mirror perpendicular to z)	xxx, $xyy = yxy = yyx$, $xzz = zxz = zzx$, $xxy = xyx = yxx$, yyy, $yzz = zyz = zzy$
Orthorhombic	
C_{2v} ($mm2$) (twofold axis parallel to z)	$xzx = xxz = zxx$, $yyz = yzy = zyy$, zzz
D_2 (222)	$xyz = xzy = yzx = yxz = zxy = zyx$
Tetragonal	
C_4 (4)	$xzx = xxz = zxx = yzy = yyz = zyy$, zzz
S_4 ($\bar{4}$)	$xyz = xzy = yzx = zxy = zyx$, $xzx = xxz = zxx = -yzy = -yyz = -zyy$
D_4 (422)	All elements are nil
C_{4v} ($4mm$)	$xzx = xxz = zxx = yyz = yzy = zyy$, zzz
D_{2d} ($\bar{4}2m$)	$xyz = xzy = yzx = yxz = zxy = zyx$
Hexagonal	
C_6 (6)	$xzx = xxz = zxx = yyz = yzy = zyy$, zzz
C_{3h} ($\bar{6}$)	$xxx = -xyy = -yxy = -yyx$, $yyy = -yxx = -xyx = -xxy$
D_6 (622)	All elements are nil
C_{6v} ($6mm$)	$xzx = xxz = zxx = yyz = yzy = zyy$, zzz
D_{3h} ($\bar{6}2m$) (mirror perpendicular to x)	$yyy = -yxx = -xxy = -xyx$
Trigonal	
C_3 (3)	$xxx = -xyy = -yyx = -yxy$, $xzx = xxz = zxx = yyz = yzy = zyy$, $yyy = -yxx = -xxy = -xyx$, zzz
D_3 (32)	$xxx = -xyy = -yyx = -yxy$
C_{3v} ($3m$) (mirror perpendicular to x)	$yyy = -yxx = -xxy = -xyx$, $xzx = xxz = zxx = yyz = yzy = zyy$, zzz
Cubic	
T (23), T_d ($\bar{4}3m$)	$xyz = xzy = yzx = yxz = zxy = zyx$
O (432)	All elements are nil

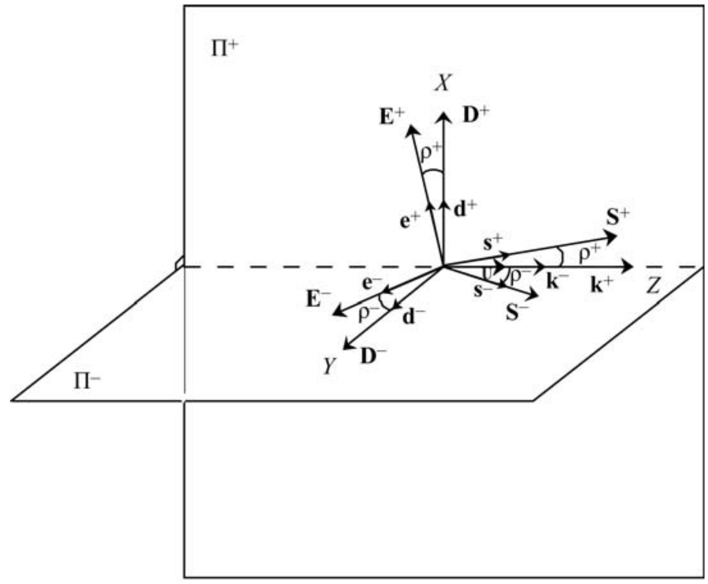

Fig. 1.7.3.1. Field vectors of a plane wave propagating in an anisotropic medium. (X, Y, Z) is the wave frame. Z is along the direction of propagation, X and Y are contained in Π^+ and Π^- respectively, by an arbitrary convention.

In the linear regime, $\mathbf{P}(\omega) = \varepsilon_0 \chi^{(1)}(\omega)\mathbf{E}(\omega)$, where ε_0 is the free-space permittivity and $\chi^{(1)}(\omega)$ is the first-order electric susceptibility tensor. Then (1.7.3.1) becomes

$$\nabla \mathbf{x} \nabla \mathbf{x} \mathbf{E}(\omega) = (\omega^2/c^2)\varepsilon(\omega)\mathbf{E}(\omega). \qquad (1.7.3.2)$$

$\varepsilon(\omega) = 1 + \chi^{(1)}(\omega)$ is the dielectric tensor. In the general case, $\chi^{(1)}(\omega)$ is a complex quantity *i.e.* $\chi^{(1)} = \chi^{(1)'} + i\chi^{(1)''}$. For the following, we consider a medium for which the losses are small ($\chi^{(1)'} \gg \chi^{(1)''}$); it is one of the necessary characteristics of an efficient nonlinear medium. In this case, the dielectric tensor is real: $\varepsilon = 1 + \chi^{(1)'}$.

The plane wave is a solution of equation (1.7.3.2):

$$\mathbf{E}(\omega, X, Y, Z) = \mathbf{e}(\omega)E(\omega, X, Y, Z)\exp[\pm ik(\omega)Z]. \qquad (1.7.3.3)$$

(X, Y, Z) is the orthonormal frame linked to the wave, where Z is along the direction of propagation.

We consider a linearly polarized wave so that the unit vector $\mathbf{e}$ of the electric field is real ($\mathbf{e} = \mathbf{e}^*$), contained in the XZ or YZ planes.

$E(\omega, X, Y, Z) = A(\omega, X, Y, Z)\exp[i\Phi(\omega, Z)]$ is the scalar complex amplitude of the electric field where $\Phi(\omega, Z)$ is the phase, and $\mathbf{E}^*(-\omega, X, Y, Z) = \mathbf{E}(\omega, X, Y, Z)$. In the linear regime, the amplitude of the electric field varies with Z only if there is absorption.

k is the modulus of the wavevector, real in a lossless medium: $+kZ$ corresponds to forward propagation along Z, and $-kZ$ to backward propagation. We consider that the plane wave propagates in an anisotropic medium, so there are two possible wavevectors, $\mathbf{k}^+$ and $\mathbf{k}^-$, for a given direction of propagation of unit vector $\mathbf{u}$:

$$\mathbf{k}^{\pm}(\omega, \theta, \varphi) = (\omega/c)n^{\pm}(\omega, \theta, \varphi)\mathbf{u}(\theta, \varphi). \qquad (1.7.3.4)$$

(θ, φ) are the spherical coordinates of the direction of the unit wavevector $\mathbf{u}$ in the optical frame; (x, y, z) is the optical frame defined in Section 1.7.2.

The spherical coordinates are related to the Cartesian coordinates (u_x, u_y, u_z) by

$$u_x = \cos\varphi \sin\theta \quad u_y = \sin\varphi \sin\theta \quad u_z = \cos\theta. \qquad (1.7.3.5)$$