Lecture 5: Polarization optics of crystals-1.

Dielectric tensor. Phase and group (ray) velocities, the wavevector and the Poynting vector. Fresnel formulas. Ellipsoid of wave normals.

In this lecture, we will consider anisotropy of optical materials, leading to birefringence and many polarization effects we already discussed and will discuss in the future. Here, we will restrict the consideration to only linear optics and will also ignore the frequency dispersion. We will also consider a non-magnetic material.

1. Dielectric tensor.

We start with the Maxwell equations. In the case of materials without induced charges and without currents, they have the form

$$\begin{aligned}
&\vec{\nabla}\times\vec{E} = -\dot{\vec{B}};\\
&\vec{\nabla}\times\vec{H} = \dot{\vec{D}};\\
&(\vec{\nabla}\cdot\vec{D}) = \rho = 0;\\
&(\vec{\nabla}\cdot\vec{B}) = 0.
\end{aligned} \tag{1}$$

Here, $\vec{H}$ is magnetization field, $\vec{B}$ magnetic field, $\vec{D}$ displacement, $\vec{E}$ electric field, and dot denotes time differentiation. In a non-magnetic material, the magnetic field is simply proportional to the magnetization field, $\vec{B} = \mu_0\vec{H}$, but the relation between the displacement and the electric field is less trivial:

$$\begin{aligned}
&\vec{D} = \varepsilon_0\vec{E} + \vec{P} = \varepsilon_0\vec{E} + \varepsilon_0\chi\vec{E} = \varepsilon_0\varepsilon\vec{E},\\
&\varepsilon = 1 + \chi.
\end{aligned} \tag{2}$$

Here, ε is the dielectric constant and χ is the susceptibility. We have ignored the nonlinear dependence of polarization $\vec{P}$ on the electric field $\vec{E}$. We will consider it in the next lectures but now, we will first sort out the anisotropy contained in Eq. (1). Indeed, we see that the relation between $\vec{D}$ and $\vec{E}$ is given by *the dielectric tensor* ε:

$$\vec{D} = \varepsilon_0\varepsilon\vec{E},$$

or, using indices,

$$D_i = \varepsilon_0\sum_j \varepsilon_{ij}E_j .$$

One can prove that the dielectric tensor is symmetric. For this, we should write the expression for the energy density of the electric field:

$$U_e = \frac{1}{2}\vec{D}\cdot\vec{E} = \frac{1}{2}\varepsilon_0\sum_{i,j}\varepsilon_{ij}E_iE_j . \tag{3}$$

From here, the symmetry follows:

$$\varepsilon_{ij} = \varepsilon_{ji} . \tag{4}$$

For a general frame of reference, there are 6 values of the dielectric tensor: $\varepsilon_{xx};\varepsilon_{yy};\varepsilon_{zz};\varepsilon_{xy};\varepsilon_{yz};\varepsilon_{xz}$. But because the energy (3) is positive, i.e., this expression is a so-called positive definite form, and it is always possible to choose such coordinates in which it is diagonal,

$$U_e = \frac{1}{2}\varepsilon_0\left(\varepsilon_{xx}E_x^2 + \varepsilon_{yy}E_y^2 + \varepsilon_{zz}E_z^2\right). \tag{5}$$

These axes x,y,z are called principal axes. In this frame of reference, the relation between displacement and electric field is simple,

$$D_i = \varepsilon_0\varepsilon_{ii}E_i, \quad i = x, y, z. \tag{6}$$

The values $\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}$ are called principle dielectric constants and denoted simply $\varepsilon_x, \varepsilon_y, \varepsilon_z$.

Importantly, dielectric constants are actually functions of the frequency (and called dielectric functions because of that); and even, in the general case, the directions of the principal axes are functions of the frequency. However, they should always obey the symmetry of the crystal. We will see this further, in the section about biaxial crystals. But in this lecture, we ignore the frequency dispersion.

It follows from (6) that the vectors $\vec{D}$ and $\vec{E}$ are parallel only if $\varepsilon_x = \varepsilon_y = \varepsilon_z$.

Eq. (5) can be rewritten as

$$U_e = \frac{1}{2\varepsilon_0}\left(\frac{D_x^2}{\varepsilon_x} + \frac{D_y^2}{\varepsilon_y} + \frac{D_z^2}{\varepsilon_z}\right). \quad (7)$$

2. Phase and group velocities.

In a plane monochromatic electromagnetic wave, all fields have space and time dependence

$$E(\vec{r},t), D(\vec{r},t), H(\vec{r},t), B(\vec{r},t) \propto e^{-i\omega t + i\vec{k}\vec{r}}, \quad (8)$$

where $\vec{k}$ is the wavevector and ω is the frequency.

From this, *the phase velocity* is directed along the wavevector and its absolute value is $v = \frac{\omega}{k} = \frac{c}{n}$:

$$\vec{v} = \frac{\vec{k}}{k^2}\omega = \frac{\vec{k}}{k}\frac{c}{n}. \quad (9)$$

Due to (8), Maxwell's equations (1) become

$$\vec{k}\times\vec{E} = \omega\vec{B}; \qquad \vec{k}\times\vec{H} = -\omega\vec{D}. \quad (10)$$

At the same time, in a non-magnetic material, $\vec{B}$ and $\vec{H}$ are parallel. Then, it follows from (10) that the three vectors $\vec{k},\vec{E},\vec{D}$ are all in the plane orthogonal to $\vec{B}$ and $\vec{H}$ (Fig. 1), and in this plane, $\vec{k}\perp\vec{D}$. But because $\vec{E}$ and $\vec{D}$ are not parallel, $\vec{k}$ is not orthogonal to $\vec{E}$. At the same time, the Poynting vector is defined as

$$\vec{S} \equiv \vec{E}\times\vec{H}. \quad (11)$$

It means that the angle between $\vec{D}$ and $\vec{E}$ is the same as the angle between $\vec{k}$ and $\vec{S}$. It is called the *angle of anisotropy*. All four vectors $\vec{k},\vec{S},\vec{E},\vec{D}$ are in the plane orthogonal to $\vec{H}$ (Fig. 1).

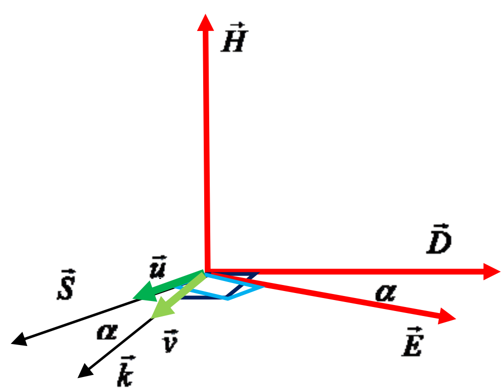

Fig.1

The total (electric and magnetic) energy density of the EM wave is twice larger than (3), because its electric and magnetic parts are equal. Therefore,

$$U = \vec{D}\cdot\vec{E}. \quad (12)$$

The *group velocity* is defined as the Pointing vector normalized to the energy density,

$$\vec{u} \equiv \frac{\vec{S}}{U} = \frac{\vec{E}\times\vec{H}}{\vec{D}\cdot\vec{E}}. \quad (13)$$

It is along $\vec{S}$ and orthogonal to $\vec{E}$ by definition; its absolute value is found from (13). Indeed, the absolute value of the numerator is EH, and of the denominator is $DE\cos\alpha$. At the same time, from the second equation in (10), $D = kH/\omega$. Then,

$$\vec{u} = \frac{\omega}{k\cos\alpha}\frac{\vec{S}}{S} \ . \tag{14}$$

We see that the group velocity differs from the phase velocity only by a factor given by the cosine of the angle of anisotropy, $v = u\cos\alpha$. There is of course additional difference due to dispersion; but we do not consider dispersion at the moment.

3. Fresnel's formulas and birefringence.

Let us derive the value of the phase velocity for a given direction of the wavevector. (We will soon see that there will be 2 values.) We take equations (10) and take into account that $\vec{B} = \mu_0\vec{H}$. Then, from the first equation, we get

$$\vec{H} = \frac{1}{\omega\mu_0}\vec{k}\times\vec{E} \ ,$$

and after substituting relation (2) between $\vec{D}$ and $\vec{E}$, the second equation becomes

$$\frac{1}{\omega^2}\vec{k}\times(\vec{k}\times\vec{E}) = -\mu_0\varepsilon_0\varepsilon\vec{E}.$$

Now, we take into account that $\mu_0\varepsilon_0 = 1/c^2$ and use the rule $\vec{A}\times(\vec{B}\times\vec{C}) = \vec{B}(\vec{A}\cdot\vec{C}) - \vec{C}(\vec{A}\cdot\vec{B})$. We get then

$$\frac{c^2}{\omega^2}\left[\vec{k}(\vec{k}\cdot\vec{E}) - \vec{E}k^2\right] = -\varepsilon\vec{E}.$$

Here, ε is a tensor, and let us write this equation in the frame of reference where it is diagonal. For each component $i = x, y, z$,

$$\frac{c^2}{\omega^2}\left[E_i k^2 - k_i\sum_j k_j E_j\right] = \varepsilon_i E_i \, .$$

Rewrite it as

$$E_i = \frac{\sum_j k_j E_j}{\left[k^2 - \frac{\omega^2}{c^2}\varepsilon_i\right]} k_i, \tag{15}$$

then multiply this equation by k_i and sum over i. We get

$$\sum_i k_i E_i = \sum_j k_j E_j \sum_i \frac{k_i^2}{\left[k^2 - \frac{\omega^2}{c^2}\varepsilon_i\right]}. \tag{16}$$

The scalar product in both sides is canceled, and we get

$$\frac{k_x^2/k^2}{1 - \frac{\omega^2}{c^2k^2}\varepsilon_x} + \frac{k_y^2/k^2}{1 - \frac{\omega^2}{c^2k^2}\varepsilon_y} + \frac{k_z^2/k^2}{k^2 - \frac{\omega^2}{c^2k^2}\varepsilon_z} = 1.$$

It is convenient to pass to the refractive index, $k = n\omega/c$, which yields

$$\frac{k_x^2/k^2}{1 - \frac{\varepsilon_x}{n^2}} + \frac{k_y^2/k^2}{1 - \frac{\varepsilon_y}{n^2}} + \frac{k_z^2/k^2}{1 - \frac{\varepsilon_z}{n^2}} = 1.$$

Let us subtract from both sides the unity, equal to $\frac{k_x^2}{k^2}+\frac{k_y^2}{k^2}+\frac{k_z^2}{k^2}$. We obtain

$$\frac{k_x^2}{\frac{1}{\varepsilon_x}-\frac{1}{n^2}}+\frac{k_y^2}{\frac{1}{\varepsilon_y}-\frac{1}{n^2}}+\frac{k_z^2}{\frac{1}{\varepsilon_z}-\frac{1}{n^2}}=0. \qquad (17)$$

This is the *Fresnel formula for wavevectors* (sometimes one says 'wave normals'). It is clear from (17) that for each direction of $\vec{k}$ its length can take two values. Indeed, multiply (17) by the product of all denominators, and we obtain

$$k_x^2\left(\frac{1}{\varepsilon_y}-\frac{1}{n^2}\right)\left(\frac{1}{\varepsilon_z}-\frac{1}{n^2}\right)+k_y^2\left(\frac{1}{\varepsilon_x}-\frac{1}{n^2}\right)\left(\frac{1}{\varepsilon_z}-\frac{1}{n^2}\right)+k_z^2\left(\frac{1}{\varepsilon_x}-\frac{1}{n^2}\right)\left(\frac{1}{\varepsilon_y}-\frac{1}{n^2}\right)=0. \qquad (18)$$

For any direction of $\vec{k}$, this is a quadratic equation for $\frac{1}{n^2}$. It follows that for any direction of $\vec{k}$, there are 2 values of n. This effect is called birefringence, or double refraction. For instance, for $\vec{k}$ along x, the solutions are $n=\sqrt{\varepsilon_y}, n=\sqrt{\varepsilon_z}$. In other words, for any direction of $\vec{k}$, there are 2 possible values of the phase velocity. For instance, for $\vec{k}$ along x, the phase velocity can be $v=c/\sqrt{\varepsilon_y}, c/\sqrt{\varepsilon_z}$.

A similar equation can be derived for the group velocity values.

4. Ellipsoid of wave normals.

There is a clear visual picture of the double refraction. Indeed, for a fixed electric energy of the wave, Eq. (7) defines an ellipsoid,

$$\frac{D_x^2}{\varepsilon_x}+\frac{D_y^2}{\varepsilon_y}+\frac{D_z^2}{\varepsilon_z}=const.$$

Passing to the coordinates $x \sim D_x, y \sim D_y, z \sim D_z$, we get the equation

$$\frac{x^2}{\varepsilon_x}+\frac{y^2}{\varepsilon_y}+\frac{z^2}{\varepsilon_z}=1. \qquad (19)$$

This surface is shown in Fig. 2. Let us choose a direction of the wavevector $\vec{k}$; the displacement vector $\vec{D}$ lies in the plane orthogonal to it. This plane intersects with the ellipsoid (19) along an ellipse (a cross-section of an ellipsoid is always an ellipse). This ellipse is shown in orange in Fig. 2. One can prove (for the proof, see Ref. 1) that the large and small semi-axes of this ellipse are along the two possible directions of $\vec{D}$ (denoted $\vec{D}'$ and $\vec{D}''$ in the figure). These are orthogonal directions. In addition, the two possible values of the phase velocity scale as the inverse lengths of these semi-axes:

$$v' \sim 1/D', v'' \sim 1/D''.$$

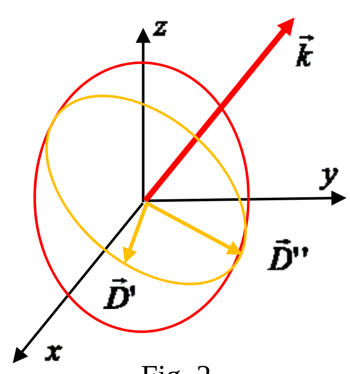

Fig. 2

Or, the refractive indices are

$$n' \sim D', n'' \sim D''.$$

We get an important conclusion: for the two possible values of the refractive index, the directions of displacement $\vec{D}$ are orthogonal. The three vectors $\vec{D}'$, $\vec{D}''$, and $\vec{k}$ form an orthogonal triplet of vectors.

One can also prove, in a similar way, that the *two possible polarization directions*, $\vec{E}'$, $\vec{E}''$, and the Poynting vector $\vec{S}$ also form an orthogonal triplet of vectors.

Optic axis or optic axes. For any ellipsoid, there are 2 circular cross sections passing through the center. (For an ellipsoid of rotation, they coincide.) Normals to these circular cross sections have the property that for them, $D' = D''$; hence $n' = n''$. Then there is no birefringence along this direction of $\vec{k}$ – this is the definition of the optic axis. Depending on the symmetry of the crystal, there can be 1 or 2 optic axes.

A more difficult task is to find the following surface: for each direction $\vec{k}$ one plots two vectors, having the two possible lengths: $k' = n'\omega/c$ and $k'' = n''\omega/c$. This is, in the general case, a more complicated surface than ellipsoid (12). In the next section we consider it separately for different types of crystals.

Literature:

1. M. Born and E. Wolf, Principles of Optics, sections 14.1-14.3.
2. R. W. Boyd, Nonlinear optics, section 2.1.