

Reflection of light by screw structures

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February 2014

We consider layers of filiform molecules which are aligned parallel to each other and parallel to the surface, where the orientation changes from one layer to the next by a small angle, leading to a screw structure. The polarizability of the molecules is anisotropic, so this structure leads to a screw structure of the index of refraction. This ordering is found in cholesteric liquid crystals and in the cuticles of some beetles.

Such layers reflect light similarly to layers with periodically changing index of refraction, with the remarkable difference that the reflected light is circularly polarized.

Calculation of the reflectivity

We assume that the surface is the plane $z = 0$ and that the orientation of the molecules corresponds to a left-handed screw. The anisotropy is described by a tensorial dielectric constant, which at $z = 0$ is assumed to be given by

$$\underline{\epsilon}(0) = \begin{pmatrix} \epsilon + \delta & 0 & 0 \\ 0 & \epsilon - \delta & 0 \\ 0 & 0 & \epsilon - \delta \end{pmatrix} \quad (1)$$

where ϵ and δ have to be obtained from experimental data on the refractive indices.

The z -dependent rotation is described by the matrix

$$\begin{pmatrix} \cos(Kz) & \sin(Kz) & 0 \\ -\sin(Kz) & \cos(Kz) & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (2)$$

with

$$K = \frac{2\pi}{H}, \quad (3)$$

where H is the pitch of the “screw”. The dielectric permittivity tensor at the coordinate z is then given by

$$\underline{\epsilon}(z) = \begin{pmatrix} \epsilon + \delta \cos(2Kz) & -\delta \sin(2Kz) & 0 \\ -\delta \sin(2Kz) & \epsilon - \delta \cos(2Kz) & 0 \\ 0 & 0 & \epsilon - \delta \end{pmatrix} \quad (4)$$

Starting point are Maxwell’s equations:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (5)$$

$$\nabla \times \vec{B} = \mu\mu_0 \vec{j} + \epsilon\epsilon_0\mu\mu_0 \frac{\partial \vec{E}}{\partial t} \quad (6)$$

$$\nabla \cdot \vec{E} = \frac{1}{\epsilon\epsilon_0} \rho \quad (7)$$

$$\nabla \cdot \vec{B} = 0 \quad (8)$$

In the present case the charge density is zero, $\rho = 0$ as well as the electric conductivity and the current density \vec{j} , in addition the magnetic susceptibility is $\mu = 1$. This leads to simpler equations. With the time derivative of Eq. (6) the magnetic field \vec{B} is eliminated:

$$-\nabla \times (\nabla \times \vec{E}) = \epsilon\epsilon_0\mu_0 \frac{\partial^2 \vec{E}}{\partial t^2}$$

With

$$\nabla \times (\nabla \times \vec{E}) = \nabla(\nabla \cdot \vec{E}) - \nabla^2 \vec{E}$$

and assuming plane waves propagating in $\pm z$ -direction with time dependence $e^{-i\omega t}$, we obtain with $\epsilon_0\mu_0 = 1/c^2$ and $\omega/c = k$

$$\nabla^2 \vec{E} + \epsilon k^2 \vec{E} = 0, \quad (9)$$

or, written in components

$$\begin{aligned} \frac{\partial^2}{\partial z^2} E_x + k^2 [(\epsilon + \delta \cos(2Kz))E_x - \delta \sin(2Kz)E_y] &= 0 \\ \frac{\partial^2}{\partial z^2} E_y + k^2 [-\delta \sin(2Kz)E_x + (\epsilon - \delta \cos(2Kz))E_y] &= 0 \end{aligned} \quad (10)$$

For numerical integration by the Runge-Kutta method, this pair of differential equations is transformed by the introduction of new variables

$$P_x := \frac{1}{k} \frac{\partial E_x}{\partial z}, \quad P_y := \frac{1}{k} \frac{\partial E_y}{\partial z} \quad (11)$$

to a set of four linear differential equations.

$$\begin{aligned} \frac{\partial P_x}{\partial z} &= -k(\epsilon + \delta \cos(2Kz))E_x + k\delta \sin(2Kz)E_y \\ \frac{\partial E_x}{\partial z} &= kP_x \\ \frac{\partial P_y}{\partial z} &= k\delta \sin(2Kz)E_x - k(\epsilon - \delta \cos(2Kz))E_y \\ \frac{\partial E_y}{\partial z} &= kP_y \end{aligned} \quad (12)$$

The quantities E_x, E_y are complex, but the real and imaginary parts are not linked by the equations (12), the equations can be integrated separately for the real and the imaginary parts. This is no longer the case if absorption is accounted for which leads to an imaginary part

of ϵ . However, numerical Runge-Kutta integration is still possible without problems.

Behind the screwy layer, at $z > L$, a homogeneous isotropic medium with refractive index n is assumed. For $z \geq L$ there can be only an outgoing wave (moving in z -direction), but its polarization is unknown. Therefore the computation is performed for two different polarizations of the outgoing wave; the choice of righthanded and lefthanded circular polarization is most convenient:

$$\vec{E}(z \geq L) = ae^{i\phi}(\vec{e}_x \mp i\vec{e}_y)e^{ink(z-L)} \quad (13)$$

This yields the boundary conditions at $z = L$ for the integration.

The integration is performed with negative stepsize from $z = L$ to $z = 0$ and yields the electric field and its derivative at the point $z = 0$ for two linearly independent solutions of the set of equations, i.e. two sets of numerical values for the quantities $E_1 \dots E_4, P_1 \dots P_4$, where

$$\begin{aligned} E_x(z = 0) &= E_1 + iE_2, & E_y(z = 0) &= E_3 + iE_4, \\ P_x(z = 0) &= P_1 + iP_2, & P_y(z = 0) &= P_3 + iP_4. \end{aligned} \quad (14)$$

In the region $z < 0$ right- and left-circular ingoing and outgoing waves are to be specified, i.e the sum of the following four terms:

Ingoing righthanded:

$$(A_1 + iA_2)(\vec{e}_x - i\vec{e}_y)e^{ikz} \quad (15)$$

ingoing lefthanded:

$$(B_1 + iB_2)(\vec{e}_x + i\vec{e}_y)e^{ikz} \quad (16)$$

outgoing righthanded:

$$(C_1 + iC_2)(\vec{e}_x + i\vec{e}_y)e^{-ikz} \quad (17)$$

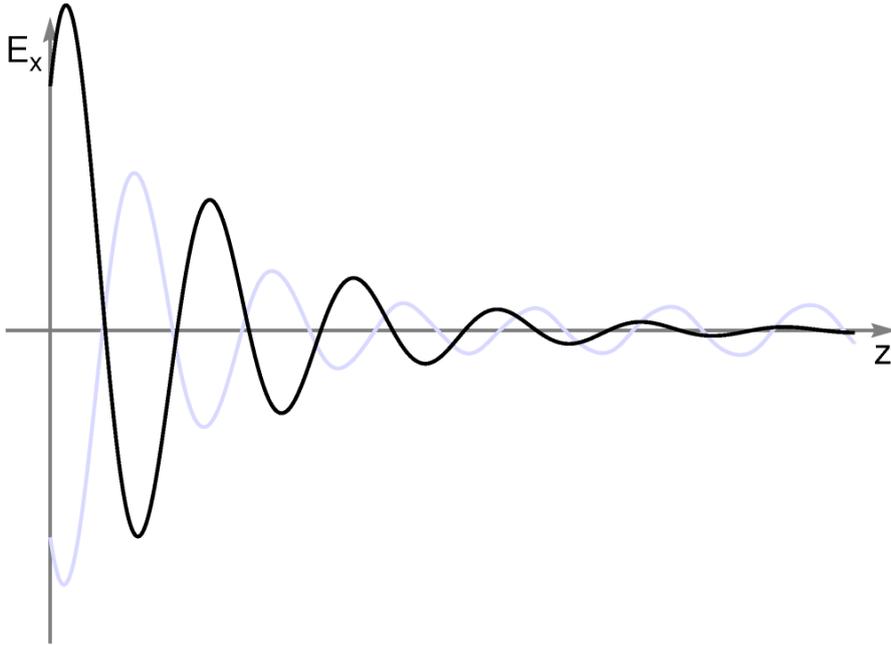


Figure 1: Integration of the wave equation in a lefthanded helical medium. Integration goes from right to left, plotted is the real part of the wave at $t = 0$. Black line: left-handed, light grey line: right-handed circular outgoing wave.

outgoing lefthanded:

$$(D_1 + iD_2)(\vec{e}_x - i\vec{e}_y)e^{-ikz} \quad (18)$$

From the continuity condition of \vec{E} and $\partial\vec{E}/\partial z$ one gets eight equations from which the amplitudes A_1 to D_2 can be determined. The

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result is

$$\begin{aligned}
 A_1 &= \frac{1}{4}(E_1 + P_2 + P_3 - E_4), & A_2 &= \frac{1}{4}(-P_1 + E_2 + E_3 + P_4), \\
 B_1 &= \frac{1}{4}(E_1 + P_2 - P_3 + E_4), & B_2 &= \frac{1}{4}(-P_1 + E_2 + E_3 - P_4), \\
 C_1 &= \frac{1}{4}(E_1 - P_2 + P_3 + E_4), & C_2 &= \frac{1}{4}(P_1 + E_2 - E_3 + P_4), \\
 D_1 &= \frac{1}{4}(E_1 - P_2 - P_3 - E_4), & D_2 &= \frac{1}{4}(P_1 + E_2 + E_3 - P_4).
 \end{aligned}
 \tag{19}$$

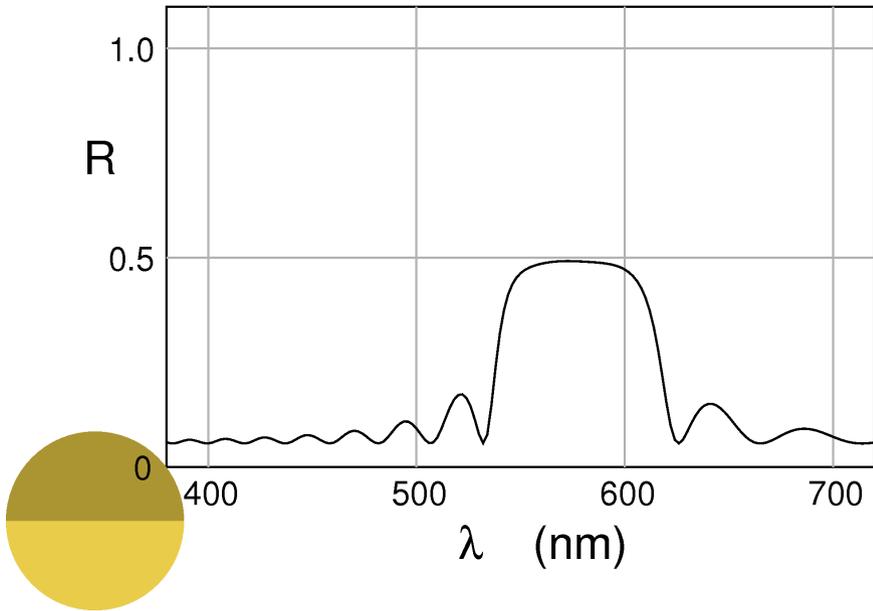


Figure 2: Reflectivity of a lefthanded helical layer for unpolarized light. Pitch of the helix: 357 nm, refractive indices: $n_{\text{parallel}} = 1.701$, $n_{\text{perpendicular}} = 1.535$, Thickness of the layer is 2856 nm. The colour sample shows the computed colour in the upper half, in the lower half the same colour with doubled brightness.

In this way we obtain two different solutions which, however, both contain left- and righthanded circular incoming waves (i.e. both are polarized elliptically). From these we can form linear combinations where the incoming waves have definite handedness. We first re-write the two solutions:

$$\begin{aligned} \vec{E}^{(1)} = & \left(A^{(1)}(\vec{e}_x - i\vec{e}_y) + B^{(1)}(\vec{e}_x + i\vec{e}_y) \right) e^{ikz} \\ & + \left(C^{(1)}(\vec{e}_x + i\vec{e}_y) + D^{(1)}(\vec{e}_x - i\vec{e}_y) \right) e^{-ikz} \end{aligned} \quad (20)$$

with

$$A^{(1)} = A_1^{(1)} + iA_2^{(1)} = |A^{(1)}| e^{i\alpha^{(1)}}, \quad \alpha^{(1)} = \arctan(A_2^{(1)}/A_1^{(1)}) \quad (21)$$

etc., and the same is done for the other solution. (The PostScript-funktion `atan` needs two arguments and yields the angle in the proper quadrant; in Fortran the corresponding function is `atan2`, `atan` yields only angles between $-\frac{\pi}{2}$ and $\frac{\pi}{2}$.)

Now the solution with left-circular ingoing wave is

$$\vec{E}^{\text{lh}} = \vec{E}^{(1)} - \frac{A^{(1)}}{A^{(2)}} \vec{E}^{(2)} \quad (22)$$

and the right-circular one is

$$\vec{E}^{\text{rh}} = \vec{E}^{(1)} - \frac{B^{(1)}}{B^{(2)}} \vec{E}^{(2)}. \quad (23)$$

The reflectivity for unpolarized light is the average of those obtained for \vec{E}^{lh} and \vec{E}^{rh} .

In the same way linear polarization of the incoming waves can be obtained; the average for unpolarized light remains the same.

Generalization for inclined incidence

Let the x - z -plane be the plane of incidence. The wave vector of the incoming wave is in the “vacuum” (air)

$$\vec{k} = k(\sin(\theta), 0, \cos(\theta)) \quad (24)$$

and the electric field has now a nonvanishing z -component. Equation (9), written in components, is now

$$\begin{aligned} \frac{\partial^2}{\partial x^2} E_x + \frac{\partial^2}{\partial z^2} E_x + k^2 [(\epsilon + \delta \cos(2Kz))E_x - \delta \sin(2Kz)E_y] &= 0 \\ \frac{\partial^2}{\partial x^2} E_y + \frac{\partial^2}{\partial z^2} E_y + k^2 [-\delta \sin(2Kz)E_x + (\epsilon - \delta \cos(2Kz))E_y] &= 0 \\ \frac{\partial^2}{\partial x^2} E_z + \frac{\partial^2}{\partial z^2} E_z + k^2(\epsilon - \delta)E_z &= 0 \end{aligned} \quad (25)$$

At first glance, this seems to be much more complicated than eq. (10), but that is not the case. The simple geometry and the boundary conditions at $z = 0$ demand that the dependence of all quantities on the coordinate x is given by the factor $e^{ik_x x}$. The only consequence is the replacement of ϵ by $\epsilon - \sin^2(\theta)$ in the equations (10). The third equation becomes

$$\frac{\partial^2}{\partial z^2} E_z + k^2(\epsilon - \delta - \sin^2(\theta))E_z = 0, \quad (26)$$

which is immediately solved analytically.

The boundary conditions are now slightly more complicated. For the wave outgoing into the substrate we write

$$A_0(\vec{e}_x \cos(\theta_0) - \vec{e}_z \sin(\theta_0) \mp i\vec{e}_y) e^{ik_0(\cos(\theta_0)(z-L) + \sin(\theta_0)x)} \quad (27)$$

with $k_0 = n_0 k$ and $n_0 \sin(\theta_0) = \sin(\theta)$. The upper sign is for right handed circular polarization.

In the region $z \leq 0$ four waves are superposed as before; incoming righthanded, incoming lefthanded, outgoing righthanded, outgoing lefthanded. These are consecutively

$$\begin{aligned}
& (A_1 + iA_2)(\cos(\theta)\vec{e}_x - \sin(\theta)\vec{e}_z - i\vec{e}_y)e^{ik(\sin(\theta)x + \cos(\theta)z)} \\
& (B_1 + iB_2)(\cos(\theta)\vec{e}_x - \sin(\theta)\vec{e}_z + i\vec{e}_y)e^{ik(\sin(\theta)x + \cos(\theta)z)} \\
& (C_1 + iC_2)(\cos(\theta)\vec{e}_x + \sin(\theta)\vec{e}_z + i\vec{e}_y)e^{ik(\sin(\theta)x - \cos(\theta)z)} \\
& (D_1 + iD_2)(\cos(\theta)\vec{e}_x + \sin(\theta)\vec{e}_z - i\vec{e}_y)e^{ik(\sin(\theta)x - \cos(\theta)z)}
\end{aligned} \tag{28}$$

From the continuity of the tangential components of \vec{E} and \vec{H} and of the normal components of \vec{D} and \vec{B} at the boundary at $z = L, x = 0$ one gets

$$\begin{aligned}
E_z &= E_{0,z} \frac{n_0^2}{\epsilon - \delta} = -A_0 \frac{n_0}{\epsilon - \delta} \sin(\theta) \\
E_x &= A_0 \cos(\theta_0) \\
\frac{1}{k} \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right) &= iA_0 n_0 \\
E_y &= \mp iA_0 \\
\frac{1}{k} \frac{\partial E_y}{\partial z} &= \pm A_0 n_0 \cos(\theta_0).
\end{aligned} \tag{29}$$

These are the starting values for the integration of eqs. (25, 26). The solution of (26) is

$$E_z(x, z) = -A_0 \frac{n_0}{\epsilon - \delta} \sin(\theta) e^{ik(\sin(\theta)x + \sqrt{\epsilon - \delta - \sin^2(\theta)}(z-L))}, \tag{30}$$

the other ones are integrated numerically as described in the previous section. Then, from the field strengths and their derivatives at

$z = 0$ the following quantities are obtained

$$\begin{aligned}
 \frac{1}{\cos(\theta)} E_x &=: E_1 + iE_2 \\
 \frac{1}{k} \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right) &=: P_1 + iP_2 \\
 E_y &=: E_3 + iE_4 \\
 \frac{1}{k \cos(\theta)} \frac{\partial E_y}{\partial z} &=: P_3 + iP_4.
 \end{aligned} \tag{31}$$

These are continuous and one can obtain the amplitudes A_1 to D_2 from them. The result is the same as that given in equations (19), and also the subsequent computations are identical.

Separation of the surface gloss from the remission of the volume

Objects which show colours due to helicoidal molecular ordering are samples of cholesteric liquid crystals and many beetles of the superfamily Scarabaeoidea, in Central Europe mainly the flower chafers *Cetonia aurata* and *Protaetia cuprea*.

In both cases the elongate molecules are approximately, but not exactly parallel to the surface. While the reflection at the surface is mirrorlike, the light reflected by the helicoidal structures in the volume is somewhat more diffuse. This makes it easy to discriminate between surface gloss and the remission from deeper layers. In the computation “ideal” conditions have been assumed, so that this distinction is not possible.

But the surface gloss can be eliminated, assuming in the region $z < 0$ there is not vacuum, but instead a medium with refractive index $n = \sqrt{\epsilon}$, so to say putting a covering glass layer on top. The angle θ , however, still refers to the waves in vacuum or air. Instead

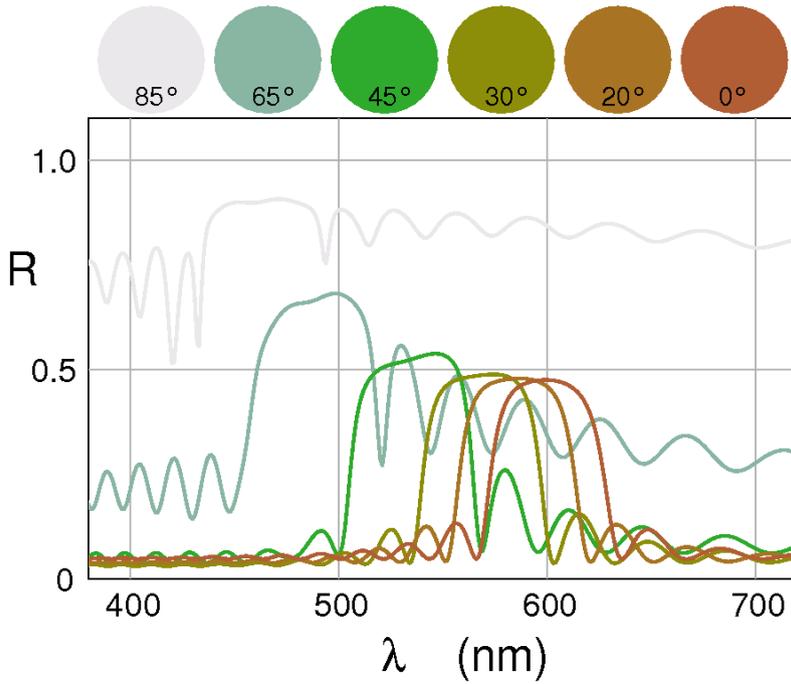


Figure 3: Reflectivity of a lefthanded helicoidal layer for unpolarized light. Pitch of the helix: 386.9 nm, refractive indices: $n_{\text{parallel}} = 1.6$, $n_{\text{perpendicular}} = 1.5$, thickness of the layer is 4000 nm.

of equations (31) one now has to use

$$\begin{aligned}
 \frac{1}{\cos(\theta_0)} E_x &= E_1 + iE_2 \\
 \frac{1}{n_0 k} \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right) &= P_1 + iP_2 \\
 E_y &= E_3 + iE_4 \\
 \frac{1}{n_0 k \cos(\theta_0)} \frac{\partial E_y}{\partial z} &= P_3 + iP_4.
 \end{aligned} \tag{32}$$

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where

$$\cos(\theta_0) = \sqrt{1 - \sin^2(\theta) / n_0^2}. \quad (33)$$

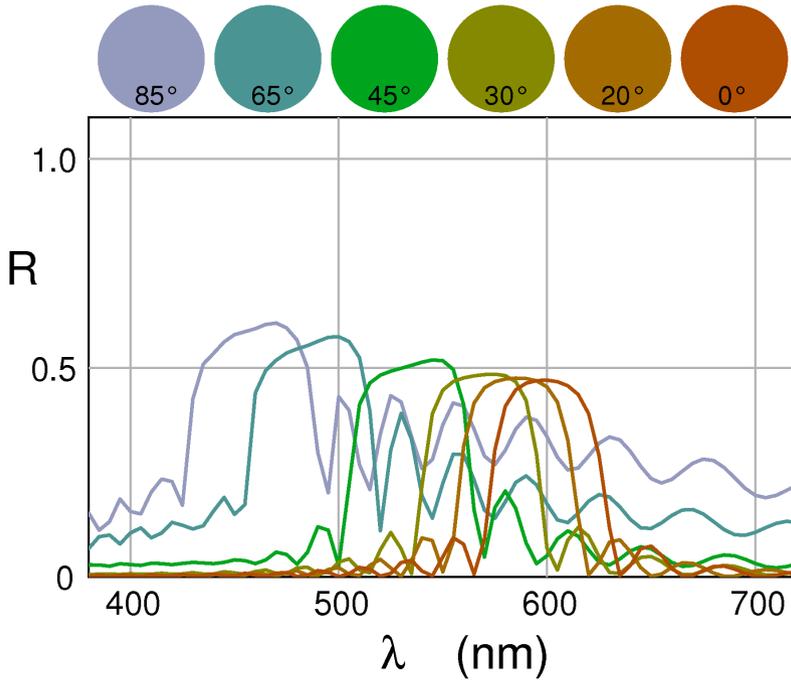


Figure 4: Reflectivity of a lefthanded helicoidal layer for unpolarized light. Pitch of the helix: 386.9 nm, refractive indices: $n_{\text{parallel}} = 1.6$, $n_{\text{perpendicular}} = 1.5$, thickness of the layer is 4000 nm. Surface gloss eliminated.