Modeling Interference Color on Surface Structured Fibers

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Abstract

A model is presented to describe color effects based on interference on approximately periodic nano-structured surfaces. The model is verified qualitatively with optical color measurements on surface structured textile fibers, which show strong iridescent color effects. Good agreement can be found for the diffracted spectra as well as on images of diffraction patterns. Furthermore we show simulations and comparisons of the color appearance of bundles of parallel fibers. This model can be used as a base for simulating color effects in textile tissues, allowing a characterization and optimization in terms of fiber cross section, structure period and type for different lighting conditions.

Motivation

The possibility to produce materials with periodic nano-structured surfaces opens new opportunities for coloring effects by light interference. It is well known that micro- and nano-scaled gratings can be used for a spectral separation of light for example to build spectrophotometers. In nature we find iridescent colors produced by periodic structures in animals (see for example butterfly[1], sea mouse[2]) and in minerals, such as opals[3]. A good review is given by Parker [4]. The physical origin for these iridescences are interference of light at thin layers or diffraction at periodic structures such as layered structures and gratings.

In the last decade or two so called photonic crystals attracted much research interest in particular in the search and production of photonic band gap material showing total reflection of light for a band of frequencies which are forbidden in this material [5]. A challenging idea is to extend material coloring beyond the possibilities of dye colors using interference effects of photonic structures. Whereas these color effects are already widely used for security elements in documents, the potential to use such color effects as a fashion element is not widely investigated. For textiles we know of one reported approach is to build regular structure into the textile fiber [6]. Another approach is to make use of the recently realized surface structuring [7]. Certain types of those fibers show strong iridescent colors. If one aims to design such textile fibers for using its color as a design element an understanding of the basic physical effect and an appropriate modeling is needed.

In this paper we describe a model which can be used as a basic for computer simulations. The goal is to allow predictions on the visual color appearance of structured textiles as a function of structure period and type, fiber cross section, material properties and illumination. In a first step the physical model is verified on spectral goniometric measurements and diffraction patterns on single fibers. In a second step the model is used to simulate the color appearance of an ensemble of parallel fibers.

Sample preparation

Different types of fibers were produced with a roll embossing technique [7], where a flexible metal stamp with a periodic pattern on the surface was mounted on a metal cylinder using a variety of process parameters. Some of them showed visible color effects. Best results were obtained for PMMA fibers. A subsequent silver coating using a plasma deposion technique [8, 9] resulted in a strong enhancement of the color effect. Two types of master stamps were used, one with a single one dimensional periodic structure (called mono-structured) and the other with a variety of microstructures (called poly-structured). The later consists of regions with different period directions each covering an area of about $1mm^2$.

A typical mono-structured fiber is shown in Fig.1. The fiber

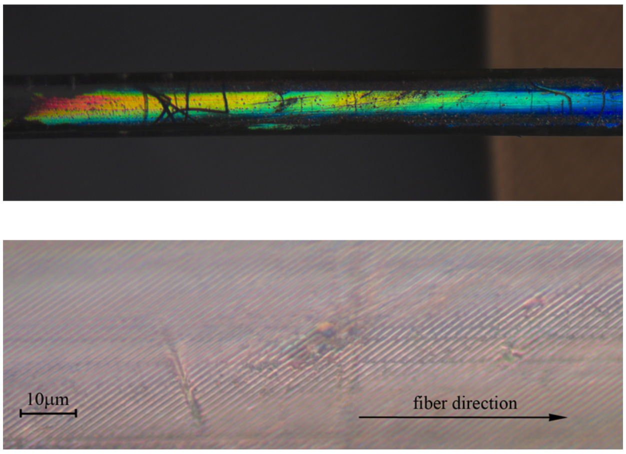

Figure 1. *Typical mono-structured fiber illuminated with white light (top) and a microscopic close up of the same fiber showing the periodic structure (bottom)*

is illuminated with white light and photographed using a light microscope. The top image shows the fiber using low magnification (50x). The bottom image shows the same fiber using high magnification (1000x). The periodic structure of about $1000nm$ can be clearly seen. Cross sections of the produced fibers have a diameter of $200\mu m$ and are of circular shape with distinct flattened regions. One example of a typical cross section is shown in Fig. 2.

Experimental methods

Spectral diffraction measurements were made with a goniometer which allowed automatic control of up to five dimensions: Angle of incident light (θ_0), detector angle (θ_1), sample inclination (α), sample rotation (β), and sample translation. For our experiments no polarizers were used neither for the light source nor the detector. For the measurement of the higher order reflections, the sample was rotated and inclined such that the

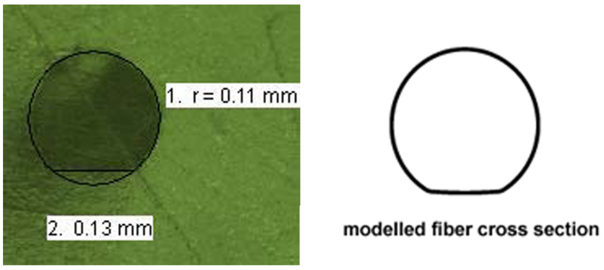

Figure 2. *Cross section of the coated PMMA fiber used for diffraction experiments: photo (left) and model (right).*

maxima of direct reflection as well as a specific higher order reflection pattern was in the plane defined by incident light and the detector arm (θ_1). The spectra were measured at different detector angles in the range of $\theta = 32-90°$ for small variation of rotation angles (β) and inclination angles(α). For an overview, photographs of the diffraction pattern projected back to a white sheet of paper were taken with common RGB-digital camera.

Model

In the literature we find various approaches to model the iridescent colors of natural objects. Some of them are based on multi-layered structures such as of Tada et. al.[10] modeling the colors of butterfly scales. Others include also periodic surface structure in their modeling [11]. Approaches to include such models for computer vision renderer were proposed by in several works [12, 13, 14]. For our model we restrict ourselves at periodic surface structures. The main goal is a physical based model to understand the dependencies of color appearance on the process parameters (fiber geometry, structure period, surface properties).

Planar approximation

The complexity of the fiber geometry and its surface structure does not allow a direct approach using diffraction grating theory [15]. Thus we propose to use a multi-scaling approach:

On the smallest scale the diffraction properties can be calculated assuming planar approximation, knowing the angle of the illumination direction with respect to the periodic structure as well as to the normal plane of the fiber surface. The basic setup is shown in Fig. 3. We use the following coordinate system: The x-axis is along and the z-axis parallel to the structure period whereas the y-axis is normal to the surface. Incident and reflected light directions are described by two angles θ and ϕ. As shown in Fig. 3 ϕ is the angle of the light with respect to the xy-plane and θ is the angle of the y-axis with the projection of the light direction onto the xy-plane. The angles θ_0 and ϕ_0 define the angles of the incident light and θ_1 and ϕ_1 the angles of the reflections allowed by the interference conditions 1 and 3

$$\phi_1 = \phi_0 \tag{1}$$

$$sin(\theta_{1,n}) = sin(\theta_0) + n\frac{\lambda}{p}\frac{1}{cos(\phi_0)} \tag{2}$$

The first interference condition is due to the translational symmetry along the z-axis and restricts all allowed reflections to be on a cone with an constant angle ϕ relative to the xy-plane. The second interference conditions is governed by the periodicity along the x-axis and restricts the allowed reflection further to distinct angles $\theta_{1,n}$ with n being the order of the Bragg reflection. For our application (visible light and period of the order of 1000nm) the orders do not exceed ± 2.

The diffraction efficiencies for the allowed reflections depend on specific surface material and shape of the structure. They can be calculated based on diffraction theory [15] using commercial diffraction grating programs [16, 17]. For all our modeling we used diffraction efficiencies for unpolarized light. This is appropriate as long as we model only single diffraction events and unpolarized lighting.

For efficiency reasons in the subsequent calculations the diffraction efficiencies were tabulated as a function of the two spherical angles and wavelength for a specific surface structure and illumination distribution.

The dimension and shape of the periodic structure was modeled by a sinusoidal shape, a period of $1040nm$ and a depth $125nm$. In this study we compare the model and measurements only for silver coated samples for which we can assume a perfect reflecting surface. In this case, the diffraction efficiencies of all reflection orders always sums to one. However it is possible to extend the model for uncoated, transparent fibers. In this case also the transmission orders into the fiber have to be considered. Then, the efficiency differences of different polarization direction have to be included in the computation.

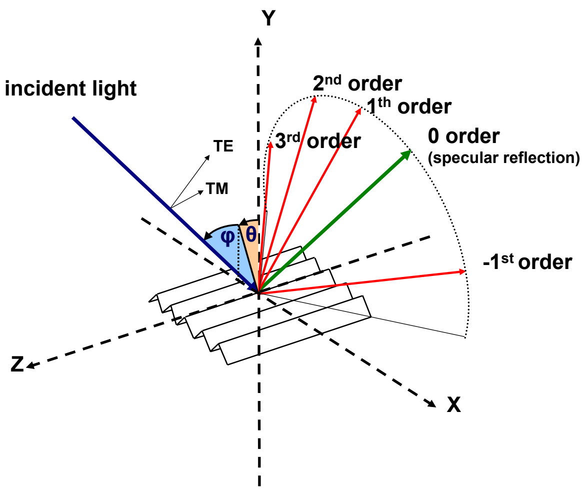

Figure 3. *Light diffraction on a periodic surface structure*

Limited periodicity

On a structured textile fiber the periodicity is limited either due to the surface curvature or the limited size of flat regions. Thus on an intermediate scale, this deviation from perfect periodicity has to be accounted for. We do this by adjusting the peak width of the reflection along the direction which is dependent on the period length. The width is inversally proportional to an average 'periodicity length'. We approximate the shape of the reflection to be Gaussian. These broadened reflections are convoluted with a Phong model[18] type description of the intensity distribution for the reflections.

Single Fibers

On the largest scale geometrical optics is used. Fibers are modeled with an arbitrary convex cross section described by a polygon with up to several thousand small edges. Every edge can either be unstructured or structured with a given period length and direction.

The geometrical setup is shown in Fig. 4 for a circular fiber sample with one flattened and structured surface. We set the x'-axis to be along the fiber direction. In the figure we show the sample where the normal $\vec{n}$ of the surface is parallel to the y'-axis. The model however allows arbitrary fiber rotations. In the general case the normal vector $\vec{n}$ is not parallel to the y'-axis. The direction $\vec{d_0}$ of the illumination as well as the direction $\vec{d_1}$ of the diffracted light are described in terms of their angle ψ_0 and ψ_1 to the y-axis and the angle ϕ_0 and ϕ_1 between the projection of $\vec{d}$ into the xz-plane and the x-axis.

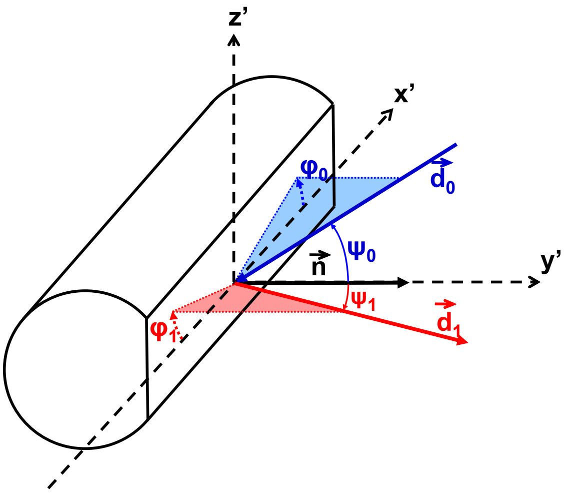

Figure 4. Geometrical setup for a single fiber modeling

The lighting is modeled by random sampling of light particles of a defined light source, which can range from directed light to isotropic lighting conditions. For every edge the coordinates system (x',y',z') is rotated to (x,y,z) so that it matches to the setting in Fig. 3, i.e. the surface normal is along the y-axis and the period direction along the x-axis. For a set of some 1000 samples the direction of the incoming light is sampled randomly from the lighting source. The intensity per unit surface area is calculated for every allowed reflection. The wavelength dependent intensity $I_{1,n}(\lambda)$ of a reflection of the order n is calculated as follows:

$$I_{1,n}(\lambda) = I_0(\lambda)cos(\psi_0)cos(\psi_1)E_n(\lambda) \quad (3)$$

where ψ_0 is the angle between the incoming ray and the normal to the fiber surface, ψ_1 is the angle between the diffracted ray and the normal to the fiber surface. I_0 is the intensity of the light source and $E(n,\lambda)$ the diffraction efficiency of the order. If one of the two angles is larger than 90° the intensity is set to zero, because the lighting or the diffraction direction would then be obscured by the fiber. The effective diffraction direction for a sample is randomly selected to model the peak broadening due to limited periodicity and surface roughness. Then the diffraction directions are rotated back from the (x,y,z) to the (x',y',z') coordinate system.

Two types of images are accumulated: The first is a diffraction image covering one hemisphere in terms of the angles ψ and ϕ. An example is shown in Fig. 5.

Furthermore a composite direct image is accumulated showing a single fiber as seen from different viewing angles ψ and *phi*. The image corresponding to Fig. 5 is shown in Fig. 6. All calculations were done for visible spectral range from 430nm to 790nm in steps of 10nm. Conversion to RGB-values were done using spectral sensitivity function of the 2-degree standard observer to obtain XYZ-values and from there the sRGB images were calculated.

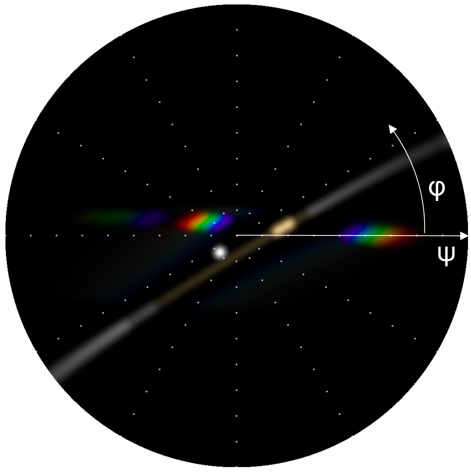

Figure 5. Simulation of a diffraction image of a typical structured fiber. It is superposed with the illumination, which consist of a white light source of a width of 2° at angles ($\psi = 10°$) and $\psi = 225°$))

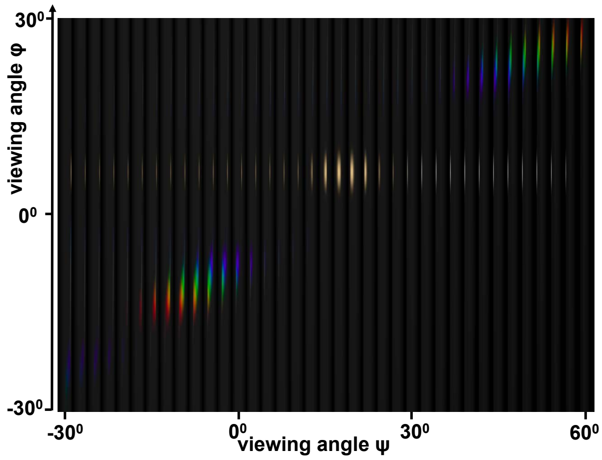

Figure 6. Simulation of direct images of a fiber seen from different viewpoints. View angles cover -30 to + 60 degree in the horizontal direction and -30 to 30 degrees in the vertical direction. The angle of periodicity with the fiber direction is 65 degrees. The illumination is the same as in Fig. 5.

Bundles

Images of arrangement of fibers can be constructed, based on a series of pre-calculated direct images of a single fiber. For a given illumination and fiber geometry we use direct images of a single fiber seen from the full viewing angles range and for a set of period direction. We show two examples for bundles of a single layer of parallel fibers. This arrangement has the advantage, that no precautions have to be made to handle hiding of one fiber behind another.

Bundles of mono-structured fibers can be constructed as follows: Fibers with random orientation are arranged side by side. Every single fiber was allowed to be slightly twisted with a random twisting angle.

For the simulation of bundles of poly-structured fibers the same basic arrangement can be used. In addition a given grain size distribution of the periodic regions can be used to select the period direction within a grain randomly.

Results

We verified our model on several levels of complexity: First by comparing spectra for selected diffraction angles, second by reproducing the color distribution of diffraction patterns and finally by modeling the color appearance of a bundle of parallel fibers. The coated PMMA fiber with the cross section shown in Fig. 2 was mounted on a spectral goniometer using a directed white beam as light source. Photographs of its diffraction pattern projected back to a white sheet of paper were taken. A sample photograph is shown in Fig. 7. The image shows the two first order reflections left and right of the direct reflection as well as the blue part of one second order reflection.

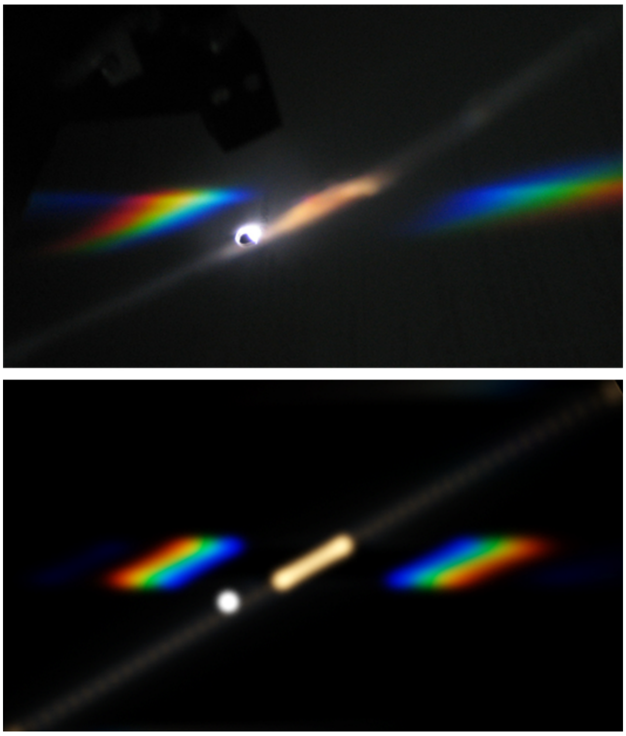

Figure 7. Diffraction pattern from a single coated PMMA fiber: photo (top) and simulation (bottom). Note that the incident light is almost perpendicular to the fiber axis. The white spot in the lower left region depicts a hole in the projection screen through which the fiber was illuminated.

Spectra were measured on a spectral goniometer in the region of the first order diffraction peak (see Fig. 8). They show the wavelength shift of the diffraction peak with the diffraction angle. The measured peak width is rather wide compared to peak width of highly periodic structures but is still small compared to human vision. In fact we can reach high color saturations even with rather wide diffraction peaks as long as they are substantially smaller than the sensitivity curves of human vision.

The general behavior of spectra (Fig. 8), as well as the diffraction pattern (Fig. 7) could be reproduced quite satisfactorily, using the known periodic structure. We used a period of $1037nm$ a depth of $125nm$ and an $65°$-angle of the period with respect to fiber direction in good agreement with the measurements made using microscope, AFM and SEM techniques. Note that even the reddish-yellowish color of the zero order reflection compared to the incoming light is in qualitative agreement with the measurement.

The color effect on a lighted bundle of fibers was simulated using arbitrary orientations of the periodic structure on the fibers. Simulations were done for mono-structured fibers as well as poly-structured fibers. For the latter the angle of the periodic pattern with respect to the fiber direction was varied randomly for fiber sections with an average length of $1mm$. In Fig. 9 the simulations were compared to photos taken for both types of structures. The rainbow type color appearance of the mono-structured fibers could be well reproduced, as well as the sparkling effect of the poly-structured fibers.

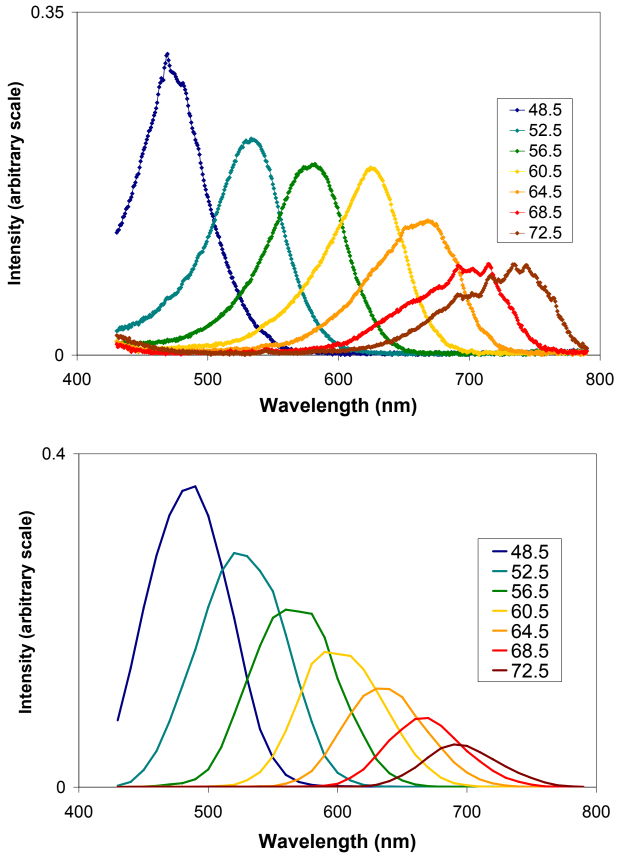

Figure 8. Diffraction spectra from a single coated PMMA fiber for selected diffraction angles in the range of $48-72°$: measurements (top) and simulations (bottom).

Conclusions

Overall, the proposed model is able to predict the general color appearance of iridescent color on structured fibers. Its strength is, that it is based on the actual physical and geometrical properties of the fiber. It allows to study the influence of fiber shape, the properties of the periodic structure and the optical surface properties. It can serve as an aid in the design of structured textile fibers for a specific application and lighting condition. However, the computational cost to describe the color appearance of arrangements of fibers exceeding simple bundle structures is too high for fast rendering. If fast rendering of more complex scenes is an issue, substantial adaptions of the model are needed to allow an integration in existing computer graphic renderers, such as the approach suggested by Sun [14].

We have shown, that the presented model can reproduce good qualitative results for the main color effects on structured textile fibers. On one hand, a further refinement of the model has the potential to be used for quantitative comparisons with spectral diffraction data. On the other hand, with a further tabulation of precompiled diffraction data, the model can serve as base for graphic simulations of tissues made of structured fibers.

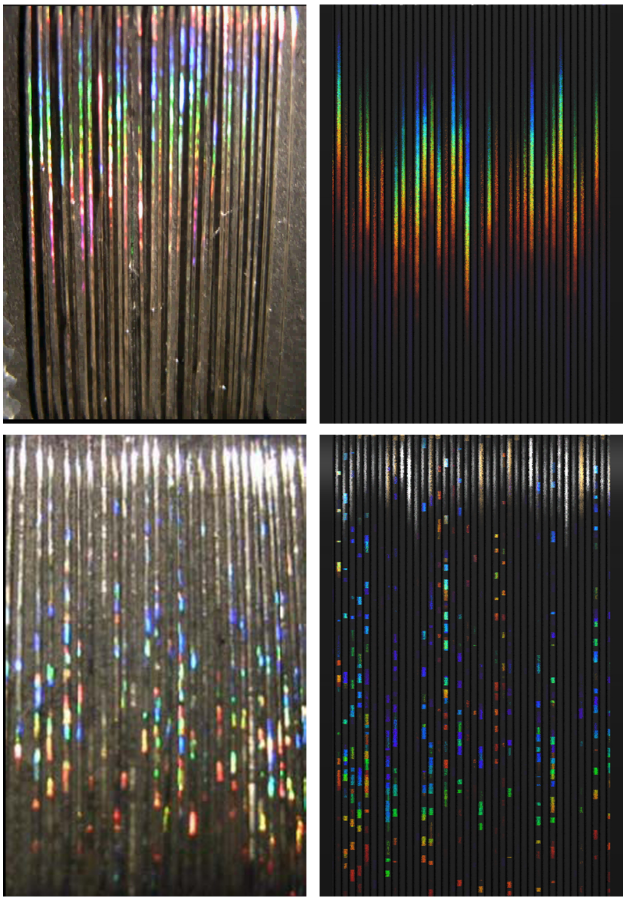

Figure 9. color appearance of bundles of parallel fibers: top: mono-structures fibers, bottom: poly-structures fibers; photos (left) and simulations (right)

Acknowledgments

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