Derivative-free optimization for optical chirality enhancement

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Abstract. We adopt a multi-objective optimization approach to design one-dimensional photonic crystals with large optical chirality enhancements. We show that this technique allows for a large design flexibility in terms of selected materials and operational wavelengths. Finally, we demonstrate that the designed platforms provide state of the art chirality enhancements above the two orders of magnitude over arbitrarily large areas and broad spectral ranges.

1 Introduction

The geometrical characteristic of three-dimensional objects that lack a mirror symmetry plane is called chirality. This phenomenon is ubiquitous at every size scale and shapes the interaction of biomolecules with their environment [1]. It is a straightforward consequence that the biochemical and pharmaceutical industries have lately focused their research effort toward a better and definitive understanding of chiral matter.

Chiral light is an excellent probe to investigate the chirality properties of a system. In particular, the adoption of left (L) and right (R) circularly polarized light (CPL) for chiroptical spectroscopy has represented the standard approach for the investigation of molecular enantiomers. Nevertheless, chiral light-matter interaction is extremely weak, especially if compared with that of standard absorption spectroscopies, which renders the study of microscopic molecular quantities extremely challenging. A promising approach suggests the adoption of specially designed electromagnetic fields to enhance the extremely weak chiroptical signals [2–5]. This can be done through the optimization of the optical chirality C of the incident electromagnetic wave, defined as $C = -\frac{\varepsilon_0 \omega}{2} Im(\mathbf{E}^* \cdot \mathbf{B})$.

A great variety of metallic and dielectric platforms have been described in the literature as a viable solution to the effective enhancement of chiroptical signals. Even so, several drawbacks such as complex fabrication or narrow spectral operation have hindered their widespread adoption. One-dimensional photonic crystals instead feature the necessary geometrical and fabrication simplicity which would make them attractive for large scale applications. Furthermore they have been already proven to be capable of supporting large optical chiralities. Yet, up to now, material and design constraints exist that need to be met in order to generate sizable superchiral fields, which complicates the fabrication process and make the platform less appealing. We adopt a derivative-free multi-objective optimization approach in order to overcome these design requirements and thus make this solution considerably more attractive.

2 Materials and methods

The structure design consists of a one-dimensional photonic crystal made by n periods of alternating low and high refractive index materials with different thickness, terminated with one final low-index termination layer. In principle, no particular constraints exist on the chosen materials or on the number of layers composing the structure, whereas in practice the fabrication feasibility of the structure in terms of complexity and material affinity must be kept in mind.

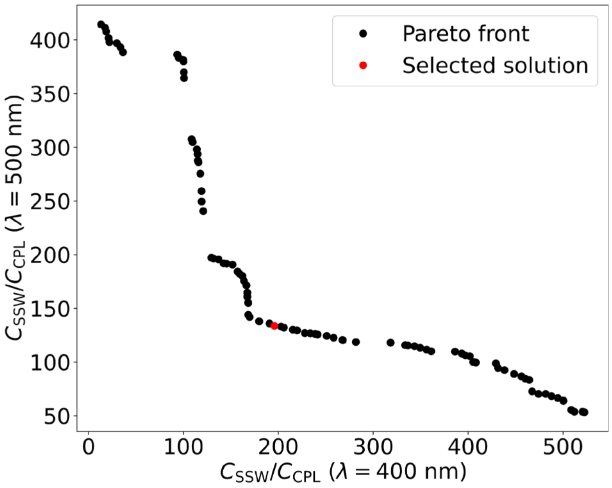

Fig. 1. Pareto front for a typical 7-layer, SiO_2/Ta_2O_5 optimization problem. Target optimization wavelengths are set at λ=400 nm and λ=500 nm for sensor operation in the visible range.

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We aim to obtain a one-dimensional photonic crystal where the transverse-electric (TE) and transverse-magnetic (TM) Bloch Surface Waves (BSW) may be simultaneously excited resulting in a surface wave characterized by a large optical chirality [6–10].

We dispense with the hand tuning of the thickness of each single layer by adopting a derivative-free multi-objective optimization approach capable of optimizing simultaneously all the layer thicknesses. In practice, we optimize the optical chirality at the photonic crystal surface at two different wavelengths, hence the multi-objective approach, and we observe empirically that this double wavelength strategy promotes the broadband alignment of the TE and TM modes [11,12].

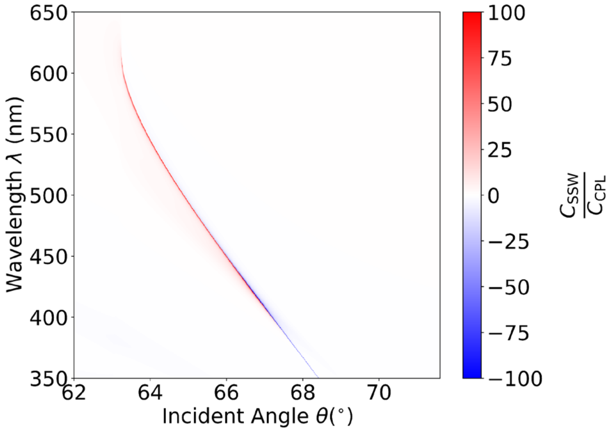

Fig. 2. Optical chirality enhancement map for the 7-layer, SiO_2/Ta_2O_5 designed solution. The structure provides two orders of magnitude chirality enhancement from λ=450 nm to λ=600 nm, covering the majority of the visible range.

3 Results and discussion

The result of a typical multi-objective optimization run, where we optimize the photonic crystal thicknesses $\mathbf{t} = \{t_1, t_2, ..., t_n\}$ to obtain maximum chirality enhancements at the design wavelengths, is reported in Figure 1. The set of all optimal solutions, represented by the black dots, forms the so-called Pareto front. In this framework, each point in the front marks an optimal multilayer configuration: points at the front boundaries are configurations that operate markedly better at one of the two design wavelengths, while points in the middle of the front represent more balanced solutions.

Figure 2 displays the (θ, λ) map of the optical chirality enhancement sampled 5 nm above the structure surface for a representative design obtained with our multi-objective optimization approach. An extremely large enhancement is visible at the superposition of the TE and TM dispersion relations over a wavelength range of hundreds of nanometers, which readily demonstrates the validity of the adopted approach. We underline that the flexibility provided by the optimization approach leads to similar results for a large variety of dielectric materials and for crystals containing from a few to several layers.

In conclusion, we showed that a derivative-free multi-objective optimization approach leads to effective one-dimensional photonic crystal designs capable of providing large optical chirality enhancements in spite of the relative structure simplicity. These results represent a step towards the realization of chiral sensing platforms for the investigation of microscopic amounts of chiral compounds.

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