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Application of Evolutionary Methods to Semiconductor Double-Chirped Mirrors Design

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Abstract. This paper reports on a successful application of evolutionary computation techniques to the computer aided design of a dedicated highly dispersive mirror which is used in an ultrafast laser. The mirror is a GaAs plate coated with many interleaving layers of GaAs/AlAs and SiO₂/Si₃N₄ layers whose thickness undergo optimization. We report and compare results obtained by leading global optimization techniques: Covariance Matrix Adaptation Evolution Strategy and Differential Evolution, as well as few efficient local optimization methods: Nelder-Mead and variable metric. The evolutionary designed mirror has been manufactured by the Molecular Beam Epitaxy technology and the measurements confirmed successful implementation of the instrument.

Keywords: CMA-ES, Differential Evolution, Double Chirped Mirror

1 Introduction

In the evolutionary computation history, it has been relatively early observed that the driving force of development of methods is their application for global optimization. Since the 1990ies, many benchmark problems have been adopted from the global optimization domain and have been used to test efficiency of evolutionary computing techniques. In 2005 and 2009, two families of benchmark sets were born: CEC [1] (starting from CEC2005) and BBOB [2] (starting from BBOB 2009). These benchmark sets include not only the test problems, but also specify procedures to test optimization methods and to interpret their results. With the use of benchmark sets it is possible to compare two optimization methods to answer the question which of them will, on average, provide better results than the other. This allows to organize competitions to select algorithms that perform most efficiently on the benchmark set.

A practitioner's perspective is somewhat different, since he/she is not interested in the long-lasting tuning of many parameters of a beloved algorithm to

make it perform better than other competitors. Instead, the practitioner is focused on obtaining an acceptable solution of a particular problem with the least effort. Results of benchmarking may be useful to perform preliminary selection of optimization methods. Parameter-free methods are obviously preferred over these with many settings to be tuned, since the practitioner is interested in easy use rather than in the development of optimization methods. Hence, software packages with predefined parameter settings will usually be preferred.

In the presented work we followed this practitioner's point of view. We report results of an application of two packages for the R environment [3], `DEoptim` [4] and `cmaes` [5], which implement DE [6] and CMA-ES [7] — two global optimization methods from the evolutionary family which have been usually on top of efficiency rankings based on benchmarking [1,8]. These methods have a relatively small number of user-defined parameters and the aforementioned packages provide default parameter settings. We applied these methods to the computer aided design of a mirror, which was dedicated for an ultrafast laser. The mirror design was represented as a vector of 126 real numbers. We have performed multiple runs of compared methods and we report statistics of the results to select the optimization method. Further tests were carried out to assess influence of starting point generation method upon mirror quality. The best structure of the mirror, which was found by the CMA-ES, was performed in a semiconductor technology and successfully tested for conformance with the design assumptions. This structure, after antireflective layer deposition, will be used to build the ultrafast laser in the near future.

2 Designing Mirrors for Ultrafast Lasers

Ultrafast lasers, which generate optical pulses in the picosecond and femtosecond range, have found numerous applications, e.g., in industry [9], biology and medicine [10]. The basic technique allowing for generation of ultrashort pulses is modelocking. We distinguish between active and passive modelocking, while the latter provides much shorter pulses [11]. The underlying principle of this technique is to induce a fixed phase relationship between the modes inside the resonant cavity. In order to achieve it, all kinds of dispersion appearing in the cavity must be compensated. This can be achieved either by using the prism pair or grating pair, or a multilayer mirror, called also a Chirped Mirror (CM) [12].

The CM is a structure that contains an alternating sequence of layers of two different optical materials. Thickness of each pair of layers is linearly variable. In effect, light from a range of wave length is effectively reflected, and longer wavelengths penetrate the structure deeper than shorter ones. Thus the delay of the reflected light depends on its wavelength. This process can be characterized by the Group Delay Dispersion (GDD) coefficient and typically, the dependence of GDD on the wavelength is very irregular, which is undesirable. This effect can be reduced in a Double Chirped Mirror (DCM) where thickness of layers is changing non-linearly. Properly designed DCM should exhibit high reflection in

a broad wavelength band together with non-oscillating dependence of GDD on the wavelength.

There are several theoretical approaches to design DCMs in an analytical way. Coupled mode theory is a perturbational approach for analyzing the coupling of vibrational systems (inter alia optical) in space or in time [13]. WKB approximation is a method for finding approximate solutions to linear partial differential equations with spatially varying coefficients [14]. For example these methods have been used by Matuschek to derive formulas for reflectivity and group delay [12]. Such analytical works undoubtedly enabled deeper understanding of chirped mirrors, but the GDD characteristics of the resulting DCM exhibited oscillatory behavior and it needed further fine tuning.

The majority of approaches to designing DCMs have used the transfer matrix method [15] to model the light reflection from multilayer structure and to optimize layers' thickness to achieve desired DCM properties. Such approach was used by Yakovlev et al. [16] who applied a memetic algorithm to design a 49-layer dielectric $\text{SiO}_2/\text{TiO}_2/\text{Ta}_2\text{O}_5$ chirped mirror. Dielectric materials were also used by other authors, e.g. Yan-Zhi et al. [17] applied a needle optimization technique [18] to design 52-layers structure with $\text{GDD} \approx -60 \text{ fs}^2$. They have also reported successful physical implementation of the design. Another successful DCM implementation has been reported by Pervak et al. [19] who used a commercial package `OptiLayer` to design a dielectric DCM for $\text{GDD} \approx -2500 \text{ fs}^2$. Unfortunately, all aforementioned articles did not report important information about optimization methods, like the objective function formulation, settings of parameters or the starting point, which does not allow to reproduce the results.

This paper briefly describes the design process of a Semiconductor DCM (SDCM). Semiconductor materials, GaAs and AlAs, which are used for the mirror realization, have high refractive indexes (3.51 and 2.95) which makes it hard to avoid reflection of the light from the mirror surface. For this reason, the SDCM should be additionally covered by an Anti-Reflective (AR) layer composed of few layers of dielectric materials. The difference of refractive indexes of GaAs and AlAs is lower than in the case of dielectric materials used by other authors, therefore more layers are needed to achieve mirror parameters comparable to dielectric DCMs. More layers means also more interfaces between layers which increases risk of harmful interferences that disrupt the GDD curve. DCMs with larger number of layers are also harder to optimize due to the "curse of dimensionality".

The SDCM production process consists of two technological stages: the Molecular Beam Epitaxy (MBE, see Fig. 1) to produce semiconductor layers on a two-inch GaAs substrate and the plasma-enhanced chemical vapor deposition technology to coat it with dielectric AR layers.

3 SDCM Design Problem Formulation

SDCM Model Mathematical model of the reflection process assumes that a time-harmonic plane wave falls on the stratified medium, which is schematically

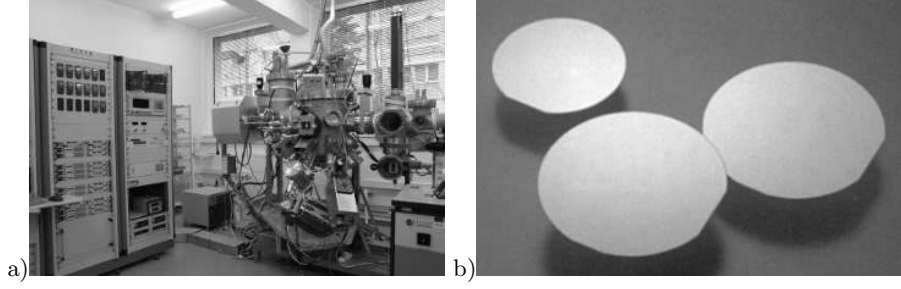


Fig. 1. a) MBE reactor which is used to produce SDCM, b) 2" substrate wafers on which the mirror is deposited

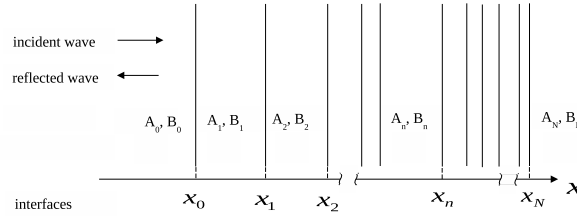


Fig. 2. Schematic view of a stratified medium

depicted in Fig. 2. The electric field $E(x)$ satisfies the Helmholtz equation [13]:

$$\frac{d^2 E(x)}{dx^2} + [(\tilde{n}_n k_0)^2 - \beta^2] E(x) = 0, \quad (1)$$

where \tilde{n}_n is the complex refractive index of the n -th layer, $\beta = n_{\text{eff}} k_0$ is the propagation constant, $k_0 = 2\pi/\lambda_0$, λ_0 is the free space wavelength and n_{eff} is the effective refractive index. In the n -th layer, the field $E(x)$ is a superposition of waves traveling towards the left and the right direction:

$$E(x) = A_n \exp(iK_n x) + B_n \exp(-iK_n x), \quad (2)$$

where $K_n = k_0 \sqrt{\tilde{n}_n^2 - n_{\text{eff}}^2}$, and A_n, B_n are constants. Assuming $A_0 = 1, B_{N+1} = 0$, we identify B_0 and A_{N+1} , as coefficients of mirror reflectivity and mirror transmission, respectively.

DCM analysis method based on the transfer matrix [15] is facilitated on the fact that the field and its first derivative must be continuous at the interfaces. According to this method we derive a matrix equation of the form:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} B_0 \\ A_{N+1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}. \quad (3)$$

Elements a_{kl} and b_k depend on thickness and refractive indexes of layers. Solution of (3) yields the key parameters of SDCM:

$$R = |B_0|^2, \text{GDD} = \frac{d^2(\arg B_0)}{d\omega^2}. \quad (4)$$

where $\omega = 2\pi c/\lambda_0$ denotes the angular frequency, c is the light velocity, R is the reflectivity coefficient, and GDD is the Group Delay Dispersion.

Representation of Solutions and Constraints On the basis of our experimentally verified knowledge it was assumed that SDCM should consist of 120 semiconductor layers and 6 dielectric AR layers. The structure is represented as a sequence of real numbers which define thickness of layers. Layers are numbered according to the sequence in which they are penetrated by the light which enters into the mirror structure. Hence, the sequence starts from AR layers, i.e. from 3 pairs of SiO_2 and TiO_2 . They are followed by 60 pairs of GaAs/AlAs. Upper limit of each semiconductor layer thickness was assumed to $0.2 \mu\text{m}$. Lower limits of thickness were 7 nm for dielectric layers and 0.6 nm for semiconductor layers, except for the the first semiconductor layer which had to be at least 30 nm thick. The first semiconductor layer is thicker to prevent the destructive oxidation of AlAs.

Objective Function The design objective was to achieve the following mirror parameters: $\text{GDD} = -2500 \pm 100 \text{ fs}^2$, $R \geq 0.999$ in a band from $\lambda_l = 1.02 \mu\text{m}$ to $\lambda_h = 1.04 \mu\text{m}$. Having performed a series of trials we decided to use the following objective function to be minimized:

$$q = a \cdot q_R + (1 - a) \cdot q_D \quad (5)$$

where q_D and q_R are the distance from the target levels of GDD and R, and a is scalarization coefficient. It is known that optimization of GDD is much harder than R, therefore a was set to 0.01. Values of q_D and q_R are defined as

$$q_D = b \sum_{\lambda} (D_0 - D_{\lambda})^2, q_R = u \sum_{\lambda} (1 - R_{\lambda})^2 \quad (6)$$

where b, u are the scaling factors responsible for bounding values of q_D and q_R in range $\langle 0, 1 \rangle$, λ is a wavelength sampled from range $\langle \lambda_l, \lambda_h \rangle$, D_0 is the required GDD value, D_{λ} and R_{λ} are the GDD and R values calculated for wavelength λ . Note that the objective function values come from the range $\langle 0, 1 \rangle$. The objective function is very irregular — sample two-dimensional cross-sections are provided in Fig. 3.

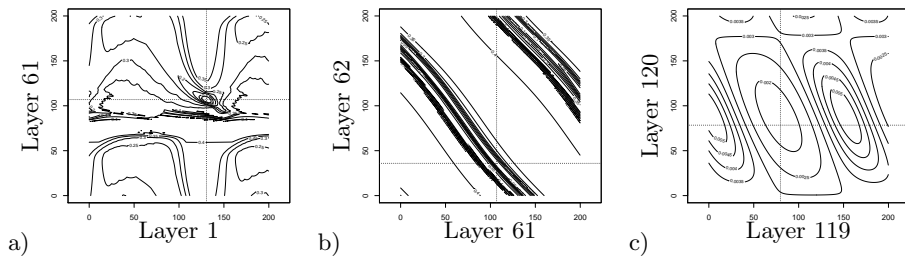


Fig. 3. Fitness function contour plot for varying thickness of: a) layers 1 and 61, b) layers 61 and 62, c) layers 119 and 120. Dotted lines marks values achieved after mirror optimization

4 Optimization of the SDCM Design

The solution of the SDCM design problem was a two stage process. In the first stage we performed experimental comparison of results obtained by several optimization methods. For all compared methods it was observed that the quality of results was unacceptable when the initial SDCM structure was set randomly with uniform distribution in the admissible area. Acceptable results were obtained when the starting structure was the design obtained by application of the theory provided by Matuschek [12]. This starting point, which will be denoted by DCM_0 , was used for selection of the best performing optimization method. In the second stage, for the selected method, different starting points were examined which finally gave the setup that would allow for obtaining high quality results. In addition to DCM_0 , we considered the Bragg mirror, which was designed to achieve high reflectivity for a single wavelength, and the single chirped Bragg mirror for which high-reflectivity bandwidth is significantly increased. Plots of the layers' thickness for these starting points are shown in Fig. 4.

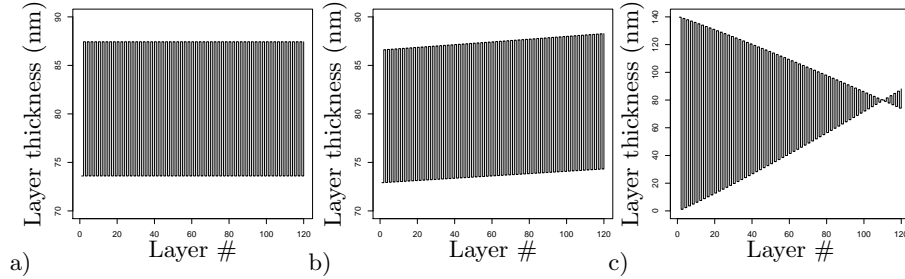


Fig. 4. Layers thickness of: a) Bragg mirror, b) single chirped Bragg mirror, c) DCM_0

Our previous experience with similar design problems [20,21] showed that metaheuristics from the evolutionary family would be good candidates for solving engineering problems. According to results of competitions [8,22] we selected Differential Evolution (DE) [6] and Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [7]. We also tested two efficient local optimization methods: nonlinear simplex by Nelder and Mead (NM), and the L-BFGS-B algorithm. The whole process of simulation and optimization of SDCM structures, and of testing optimization methods, was performed under the R environment [3]. We used R packages: `cmaes` for the CMAES [5] and `DEoptim` for the DE [4]. Implementations of NM was provided by Bihorel et al. [23] and L-BFGS-B [24] was taken from the `optim` package.

Selection of the Most Efficient Optimization Method In preliminary tests we observed that DE was able to improve the quality of the initial design using default parameter settings but the GDD spectral characteristics was far from

satisfactory. Default parameter settings for CMA-ES yielded no improvement to the initial design. Therefore we performed manual parameter tuning and we ended up with different settings which gave acceptable solutions. In the case of CMA-ES, Hansen suggested [25] that in most cases default values of parameters which are used by the "reference" implementation of CMA-ES should be appropriate if design variables are scaled to fit into the range $\langle 0, 10 \rangle$. Our design variables are bounded by 0.0006 and 0.2, so they are not in CMA-ES "favorite" range. Instead of scaling, we changed the σ parameter and we observed good results for $\sigma = 0.0003$. We used the default DE version in the `DEoptim` package, which was the DE/local-to-best/1/bin algorithm. The best results were obtained for CR=1 and the remaining parameters were set to the default values. The DE method must be started with a diversified population. To achieve this, the initial population was filled with Gaussian perturbations of the starting point.

An additional comments needs to be made on the NM method. We tested its three different implementations: NM₁ [26], NM₂ [23] and NM₃ from the `optim` package. These three versions gave substantially different results: NM₁ was 10 times worse than NM₃ and 33 times worse than NM₂. For this reason we report only the results by NM₂.

In Fig. 5a, box and whisker plots are provided of the distribution of the best objective function values obtained in 25 independent runs of compared algorithms; for NM and L-BFGS-B a single value is provided, since they are deterministic methods and the starting point is always the same.

According to the results, both DE and CMA-ES outperformed their competitors when starting from the initial design DCM₀. CMA-ES revealed greater variability than DE, but in the same time median of its results was significantly better than for DE. For this reason, an additional experiment was made to check if the CMA-ES efficiency could be further improved by using a different starting point.

Sensitivity to the Starting Point From preliminary experiments we learned that the CMA-ES was unable to generate acceptable solutions when started from a random solution. The DCM₀ structure is a nearly optimal design which introduces a risk that it would become a trap which would not allow CMA-ES to generate better solutions which are substantially different than the initial structure. In Fig. 5b we provide statistics of objective function values achieved for 25 independent runs of CMA-ES for three starting points depicted in Fig. 4. The DCM₀ structure appeared the worst among all considered starting points, although this structure is the result of the most advanced analytical approach to the DCM design. Much better results were obtained for simple Bragg and linearly chirped mirrors — in most of runs CMA-ES was able to approach the global minimum of the fitness. For the single chirped structure the number of successful runs was greater so we conclude that this was the best choice of starting point for CMA-ES.

Solutions generated from this starting point revealed another advantage over those generated from DCM₀. According to the technology experts, they were

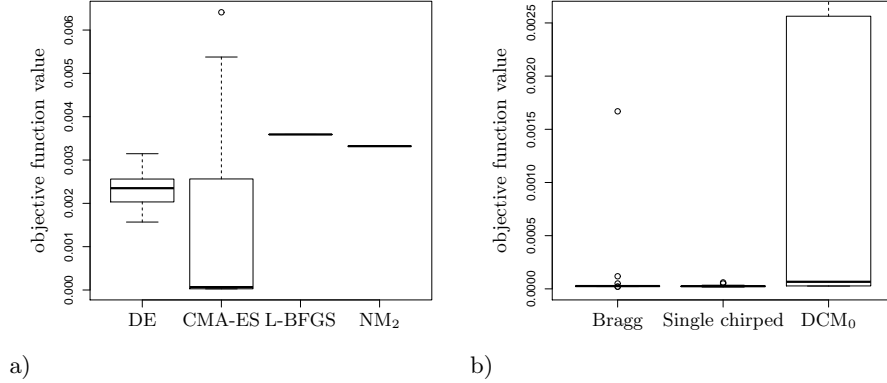


Fig. 5. Box and whisker plots of the best objective function values obtained in 25 independent runs of each method; a) Results for various optimization methods with starting point DCM₀, b) results of CMA-ES for three different starting points

easier to produce, because thickness of neighboring layers is less diversified. Another advantage of obtained designs was that they allowed for reduction of the number of layers. We took the best result obtained in all experiments and we removed 10 semiconductor layers and 4 dielectric layers (in both cases layers were removed from the base side). Additionally we changed TiO₂ dielectric into Si₃N₄. This was the starting point for CMA-ES which yielded another solution that satisfied design criteria. This solution was the final design (see Fig. 6a).

5 Implementation and Tests of the Designed Mirror

The final design obtained by CMA-ES was used to produce the semiconductor part of the mirror in the MBE reactor (Fig. 1) in the Institute of Electron Technology (ITE). Prior to coating the mirror with AR layers, its R and GDD factors were measured by the ITE and Institute of Experimental Physics in the assumed wavelength band.

Measurements of GDD were performed using a modified Michelson interferometer illuminated with a white light source, delivered by a halogen bulb, to obtain GDD characteristic in a broad range of wavelengths. A reference curve of GDD vs. wavelength has been generated from the SDCM model and it was verified if it is approximately matched by the measured curve. The results, which are presented in Fig. 6b, indicate a good agreement of both curves.

Mirror reflectance was measured using a dark configuration of a standard optical set-up, where a broadband source light is dispersed by a monochromator and formed to a quasi-parallel probe beam which illuminates the sample surface at normal incidence. Reflected light is optically collected and focused onto a silicon detector. The measurement confirmed that the mirror reflectance matched the design criteria.

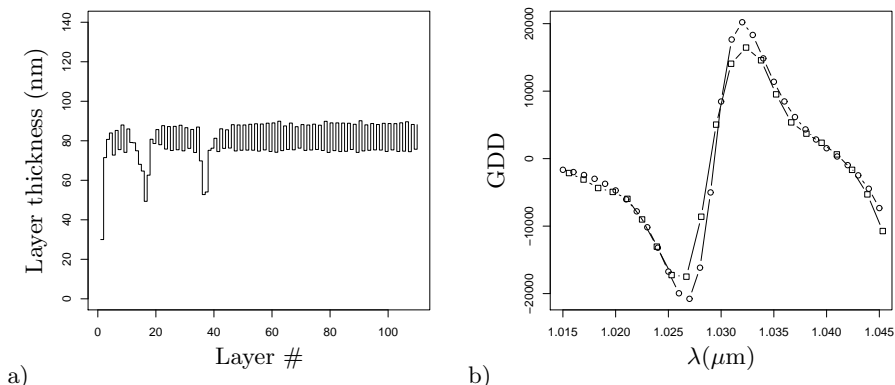


Fig. 6. a) Layers thickness of designed SDCM. b) Comparison of theoretical (circles) and measured (squares) GDD characteristics

The measurements confirm that the mirror was correctly produced by the MBE process, and it therefore can undergo the second phase of production – deposition of 2 dielectric layers of AR coating. The resulting product will be used as a component of an ultrafast laser constructed by Institute of Experimental Physics.

6 Conclusions

We presented a successful practical application of evolutionary techniques to the design of a Double Chirped Mirror which was produced in the semiconductor technology. Application of CMA-ES yielded a solution that outperformed engineering practice of designing DCM structures. Obtained design was also acceptable from the production technology point of view. The mirror has been performed and it will be used to build a compact ultrafast laser.

The design problem size exceeds an informal limit of 100 dimensions which was suggested for CMA-ES applications. Quality of obtained results is sensitive to the starting point which indicates that analyzed methods realize a form of a “globalized local search” — they are only partially robust against getting trapped into local optima. The objective function used for the design, which has been implemented in the R language, is very irregular and it may serve as a benchmark problem for testing global optimization methods.

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