Aperiodic thin film filters for acoustic phonons

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Abstract. We describe multilayer acoustic nanowave devices based on aperiodic stacks of GaAs and AlAs layers and achievable with standard Molecular Beam Epitaxy (MBE) technology. These nanostructures were designed to display optimized acoustic reflectivity curves in the terahertz range. We address the design and optimization of these devices using a downhill simplex algorithm. We analyze different strategies of optimization, and we study the different engineering parameters relevant for the conception of aperiodic filters.

1. Introduction
Acoustic phonons can be used as sensitive nanoscopic probes of thermodynamic phases, piezoelectric fields, and electronic states and for nanostructure characterization. Several applications in the field of phononics can be envisaged where the control and manipulation of vibrational fields is a main concern. Many times inspired by the field of optics and photonics, devices based on phononic crystals have been developed during the last ten years, for example: mirrors, [1, 2], cavities, [3, 4, 5] phononic lenses, [6] waveguides, [7] and demultiplexers, [8, 9] to name a few.

Based on their optical equivalents, in this work we address the problem of the design and optimization of aperiodic thin film phononic filters, operative in the THz range. State of the art in molecular beam epitaxy (MBE) of semiconductor and oxide materials (GaAs, AlAs, SrTiO\textsubscript{3}, BaTiO\textsubscript{3}, etc) allows growing samples with interfaces with resolutions up to one atomic monolayer, reaching the required accuracy for THz vibration control and applications. In what follows we describe routines and strategies for the design and optimization of aperiodic phonon filters. We present the results of an edge filter and a color filter.

2. Design and optimization of acoustic thin film filters
The conception and design of complex aperiodic devices requires the solution of an inverse problem, that is the determination of the distribution of the layer thicknesses in a nonperiodic multilayer, that corresponds to a specific acoustic reflectivity. As multidimensional optimization tool we used the Nelder and Mead (NM) downhill simplex routine. [10] The reflectivity is computed by solving the sound wave equation in each layer and matching strain and displacement...
The first design is an edge filter. It is a device that has a high transmission below a well defined energy edge, and high reflectivity above it. In Fig. 1 (left) we show the calculated reflectivity for an optimized edge filter and a periodic multilayer for comparison purposes. In the low energy region, the reflectivity is less than 1% in all the optimized range. On the other hand, in the high energy region the stop-band is the same as in the case of a periodic structure. The optimization was performed using a periodic 80 layer GaAs/AlAs 6.56/2.61 nm SL seed to obtain an edge filter $F_A$. $F_A$ was conceived to have a high transmittance from 15.3 cm$^{-1}$ to 17.4 cm$^{-1}$ and high reflectivity in the 17.5-18.5 cm$^{-1}$ region. In the lower panel (left) we show the thickness deviation of the optimized device from the periodic SL. The larger variations occur at the beginning and end of the device.

Color filters are devices with characteristics of selective transmittance, capable of passing a certain part of the spectrum while being highly reflective to the other portions. Figure 1 (right) shows the calculated phonon reflectivity and corresponding thickness deviation from a periodic SL for an optimized 160 layer GaAs/AlAs structure (shown in the lower panel). The transmission band was set in the 16.95-17.45 cm$^{-1}$ region. The design of the optimized color filter was performed in a two step optimization process. [12] The first step consisted in two independent optimizations: a periodic 80 layer GaAs/AlAs 6.56/2.61 nm SL was used as a seed to obtain a filter $F_A$, being the same as in the case of the edge filter. We designed a second filter $F_B$, optimized to have a high transmittance region in the desired band, but a high reflectivity band between 15.95 and 16.90 cm$^{-1}$. In the first stage of the optimization, to generate $F_B$ we used no seed, i.e., all vertices in the simplex were random structures. The second step consisted in the optimization of the desired color filter using the $F_B + F_A$ 160 layer structure as seed. Using the outlined optimization scheme, it is possible to fix the transmission region just changing the positions of the individual seed filters $F_A$ and $F_B$. Note that the larger variations occur at the $F_B$ part of the sample, due to the random origin of this filter.

The studied one-dimensional multilayered nanostructures present reflectivity curves that are almost periodic with the thickness of each layer. Figure 2 shows how the objective function value changes with the thicknesses of the layer 15 (GaAs), and layer 16 (AlAs). In this plot darker regions represent lower objective function values, and therefore better responses of the candidate structure. The points A and B indicate two structures with similar performance.
Each layer has associated a phase $e^{ikd}$, where $k$ is the acoustic wavevector and $d$ the layer thicknesses, [5] so every layer has associated a period $T=2\pi n/k$ with $n$ an integer number, that leaves this phase almost unaltered for a limited energy band. Using this characteristic of the multilayer filters, it is possible to change some critical thicknesses without changing significantly the performance of the optimized device. This can be useful, for example, in applications where electronic resonances of the quantum wells must be taken into account (e.g., in the Raman scattering characterization of the samples and if optical transparency is required).

It is interesting to note that it is also possible to shift the reflectivity curve, just proportionally changing all the thicknesses. In fig. 3 we show the calculated acoustic reflectivity of the optimized edge filter, and the effect of increasing (decreasing) the layer thicknesses by an amount of 40%. The grey regions indicate the optimized energy band. Note that the width of the optimized band is proportional to its energy. The possibility of moving the operative band of the devices allows to use a single optimization result for several energy ranges. Nevertheless, attenuation effects might be relevant for certain applications and energy ranges. In these cases, a new optimization might need to be performed for every energy band. In the case of the color filter, making a proportional change of all the thicknesses of $F_A$ and/or $F_B$ before the last optimization step is an easy way to change the transmission region of the device.

An alternative set of optimization parameters is the acoustic impedance of the layers, defined as the product of the density and the velocity of sound. This can be done, for example, changing the content of Al in an AlGaAs alloy. To illustrate the strategy we conceived an edge filter as an Al$_x$Ga$_{1-x}$As multilayer, with $x$ different for each layer, and the thicknesses forming a periodic array. The only free optimization parameter was the content of Al in each layer. Fig. 4 shows the achieved acoustic reflectivity and the distribution of Al content throughout the structure. We used a 6.56/2.61 nm GaAs/AlAs 80 layers SL as seed, and the rest of the vertices of the simplex were identical structures but with the GaAs (AlAs) layers replaced by Al$_x$Ga$_{1-x}$As with $x < 0.15$ ($x > 0.85$). It can be observed that the edge is slightly shifted. This could be due to the modification of the effective impedance mismatch and the departure from the optimal $\lambda/4-3\lambda/4$ thickness relation. [13] This relation optimizes the first zone center minigap (important for Raman scattering experiments and coherent optical generation).
As it was already stated, it is possible to use seeds to accelerate the convergence of the optimization process [12]. Figure 5 shows the objective function value for the edge filter as a function of the iteration number for different conditions of the initial simplex. The curves labeled Rnd correspond to the case where all the vertices of the simplex are random structures with layer thicknesses between 0 and 10 nm. The second studied initial condition consist in introducing only one seed, and leaving the rest of the vertices are random structures (marked as seed in the figure). Finally, we have considered a case where one seed is introduced, and each of the other vertices is generated by taking this seed and randomly varying each layer thickness up to 10% (noted as S10 in the figure). The latter case describes an initial (small) simplex defined around the original seed. It is this method the one that presents the fastest convergence. The Seed cases also shows a rapid convergence, although the reached objective function values after 10000 iterations is worse than in S10, probably reaching sufficiently good local minima. The option without seeds, with an initial random simplex has the worst performance, and in some cases the simplex falls in a local minima giving an unuseful result.

3. Conclusions
We discussed the design and optimization strategies of acoustic devices using non-periodic structures. The implementation of the NM optimization algorithm have demonstrated a procedure to obtain phononic devices operative in the THz range, structures that are growable with standard molecular beam epitaxy (MBE). We found that in the optimization of devices, it is convenient to use intelligent seeds, in order to reduce the parameter space and accelerate the convergence. The described methods and routines can be easily applied in the design of other phononic devices, such as mirrors, notch filters, multiple pass band filters, etc. Alternative strategies can be implemented to optimized layered unit cells for desired bandgap characteristics. [14] New applications of the optimization strategies developed during this work can be envisaged. In particular, the extension to the design of novel phononic tools, such as tailored sounds sources in ultrafast laser pump-probe techniques.

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