Effects of top layer inhomogeneities on the performance of Fabry-Perot cavities and open resonators based on distributed Bragg reflectors

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ABSTRACT

Optical and acoustic resonators utilizing distributed Bragg reflectors (DBRs) are pivotal in advancing technologies ranging from lasers to quantum computing. Under ideal, smooth interface conditions, the efficiency of these resonators, quantified by their quality factor, primarily depends on the number of DBR pairs. However inhomogeneities of the top layer thickness commonly occur, either during growth or fabrication, and is even more severe when a dielectric material is deposited on the top of the samples, for example in responsive resonators. This study analyzes the effects of such inhomogeneities on the resonators' quality factor in the case where the nanometer-scale vertical dimension of the inhomogeneities is significantly shorter than their lateral scale. Employing an analytical approach, we demonstrate that such inhomogeneities can significantly degrade the quality factor, imposing a practical limit to its enhancement irrespective of the DBR pairs added.

Keywords: thickness inhomogeneities, distributed Bragg reflector (DBR), DBR resonator, quality factor, open cavity, Fabry-Perot resonator

1. INTRODUCTION

Distributed Bragg reflector (DBR) devices based on semiconductor heterostructures are pivotal components in both fundamental and applied fields of photonics and nanophononics. A pair of DBRs enclosing an optical spacer constitutes a Fabry-Perot optical cavity, capable of shaping the optical local density of states. Over the past three decades, such optical cavities have been used in a plethora of applications encompassing quantum technologies, optoelectronics, photonics, and spectroscopy.[1–14] Similarly, acoustic cavities utilizing the same DBR configurations can confine and enhance phononic fields, offering prospects for ultra-high frequency applications.[15–17] Furthermore, these cavities were recently used in optomechanics, and as platforms for simulating solid-state physics phenomena.[18–26]

The widespread use of DBRs and their resonant structures emphasizes the importance of developing accurate tools for optimized device design. Current designs and evaluations of optical and nanophononic devices often focus solely on the number of DBR periods and materials.[27] However, the reality of material growth and fabrication always entails some surface roughness, even in samples produced using cutting-edge techniques. While the roles of interface roughness[28] and fabrication defects[29] were analyzed in specific instances, the impact of surface thickness variation and surface roughness are commonly overlooked, presumably due to the assumption that their influence might be negligible. To justify this conjecture, one would have to assume surface roughness of negligible magnitude, combined with the fact that the confined mode is mainly localized within the cavity spacer. However, in reality, some variations of the top layer thickness often occur during device processing, or due to oxidation of the top layer of structure. Additionally, some degree of surface roughness is invariably present even when using state-of-the-art growth techniques.[30–32] These factors may play an important role in specific structures, such as DBR resonators, which rely on precise definition of the multi-layered structure to define the resonant frequencies.

In this study, we investigate the effects of variations in surface roughness on the performance of DBR-based resonators. Our analysis emphasizes their influence on both phonon and photon dynamics, as well as on the

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quality factor (Q-factor) — a crucial metric that quantifies energy dissipation in these resonators. We center our investigation on GaAs/AlAs DBR superlattices, examining both acoustic and optical micro-cavities, specifically, Fabry-Perot (FP) and open-cavity resonators. Our analysis highlights the notable impact that even slight changes in the top layer thickness and roughness can have on the Q-factor.

2. MODEL IMPLEMENTATION

To simulate the structure, we employ a model based on the transfer matrix method (TMM). We consider free-strain boundary conditions and solve the standard 1D wave equation. Detailed implementation specifics of the TMM for studying transmission and reflectivity spectra in multi-layered superlattices are outlined in.[33,34] We here extend this method to account for surface roughness, introducing a simplified model that simulates the effects of roughness on acoustic FP and open cavity resonators. Surface roughness can have various sources, resulting in either more (additive roughness) or less (subtractive roughness) material than originally designed. In GaAs/AlAs structures additive or subtractive roughness may arise during material growth or device processing, and as a result, it can vary in terms of its type and direction.

For example, a relatively small variation on the order of one monolayer (ML) ($\sim 0.5nm$), is commonly observed in high-quality epitaxially grown flat layers, such as MBE-grown GaAs/AlAs or InGaAs/InP structures.[30,31,35] This roughness tends to be discrete, usually resulting in 1-ML-thick plateaus in the lateral direction. Non-flat layers, like quantum dot (QD) nanostructures, frequently integrated within DBRs due to their exceptional optical and quantum properties, might contribute to nm-scale roughness in the layers grown on top of them. Larger roughness is expected when an additional layer is placed atop the MBE-grown cavity, or for samples grown using different techniques. In such cases, the roughness can vary significantly based on the specific technique and material, typically ranging from a few nanometers to a few tens of nanometers. Furthermore, additional roughness or width variations of the top layer might arise due to oxidation,[30] or during device fabrication processes, such as etching or mask removal steps. This roughness' texture is random and continuous in the vertical direction, and it varies from sample to sample.

In this work, we have developed and implemented a simplified model that approximates the roughness of one sample as a set of samples that exhibit planar surfaces and different thicknesses, averaging their simulated surface displacements. Specifically, we model the surface roughness by considering a normal distribution of thickness variation for the top layer of the structure, with a standard deviation σ. For each case, we average the resulting spectra over 2000 iterations of random thickness distributions with a specific σ, while keeping the parameters of the other layers of the DBR constant. Subsequently, we fit the resonant modes using a Gaussian function and calculate the Q-factor by computing the ratio between the resonant frequency and the linewidth extracted from the fitting. This model is valid when the lateral roughness profile is much larger than the phononic wavelength, which is the case we consider in this work. As a result, scattering and interference effects due to lateral modulation of the roughness may be neglected. Unless explicitly stated differently, we imply this averaging process when we refer to roughness simulation in this paper.

In the outlined approach, we work under the assumption that the inhomogeneous broadening approximation remains valid. Specifically, surface roughness introduces inhomogeneous broadening of the resonant modes, which influences the resonator's response and compromises its Q-factor. The studied structures are based on GaAs/AlAs DBR superlattices with flat interfaces, finalized with the top layer which contains a rough surface. The periodicity of the superlattice introduces Brillouin zone folding and miniband openings at frequencies $\Omega_m = m\pi v/d$, where $m \in \mathbb{N}$, and d and v represent the unit cell thickness and phonon group velocity, respectively.[17,36,37] Throughout our analysis, we consider appropriate thickness inhomogeneity ranges, taking into account the typical values observed in practical samples. The material parameters for GaAs, AlAs and alloys utilized in our analysis, are drawn from relevant literature sources.[30,38]

3. RESULTS

Our study begins with an analysis of how variations in the top layer inhomogeneities impact the response of Fabry-Perot and open resonators. These fluctuations in top layer thickness are common in practical samples and can arise due to processes like oxidation of the top layer upon exposure to the atmosphere,[30] or during device

fabrication steps such as etching or mask removal .[7] Schematics of the investigated resonators are presented in Figure 1(a,b).

The first structure (Figure 1(a)), is a conventional FP cavity, incorporating a $\lambda/2$-cavity between two GaAs/AlAs DBR superlattices, with λ representing the acoustic wavelength. This configuration results in a high-quality cavity for both photons and phonons due to the nearly identical refractive index contrast and acoustic impedance contrast of GaAs and AlAs.[39] Moreover, the closely matched lattice constants of these materials facilitate the growth of thick, high-quality layers using standard epitaxial techniques, making them ideal for applications involving high Q-factor microcavities.

The second design under investigation is the open-cavity resonator (Figure 1(b)), formed by a $3\lambda/2$ low-acoustic-loss spacer cavity on top of a single DBR. In the absence of surface roughness, in this arrangement, the free surface acts as a perfect mirror for phonons at the studied frequencies, since they cannot propagate toward the air. Consequently, when combined with a high-reflection bottom DBR, this arrangement generates a cavity with a high Q-factor, rendering it an ideal platform for our investigation.

We performed a study of the parameter space to assess the effects of the top layer thickness inhomogeneities on the quality factor, focusing on the case where the vertical dimension of the roughness is much smaller than the lateral one. This simplification has allowed us to simplify the model substantially. We acknowledge that while being precise for this particular type of roughness, to fully account for the most general type of roughness in which both vertical and lateral dimensions are of nm-scale, we would need to employ a full 3D model. However, we do believe that the main trends and conclusions that we reach in this paper, will still hold in this case as well. For brevity, from this point forward in this paper, we will refer to this type of top layer thickness inhomogeneities as roughness. In all configurations, we maintain a constant difference of 4 GaAs/AlAs layer pairs between the top and bottom DBRs. This difference ensures a symmetric optical cavity due to the higher refractive index contrast at the DBR/air interface compared to the DBR/substrate interface.

Figure 1(c) focuses on Fabry-Perot resonators, analyzing five configurations with varying numbers of periods in the bottom DBR (ranging from 5 to 25 in 5-bilayer intervals). In all cases, the top DBR comprises 4 periods less than the bottom DBR (1, 6, 11, 15, and 21). Corresponding results for open cavities are shown in Figure 1(d). The two key parameters —roughness and the number of DBR layers— exert a pronounced and predictable influence on the Q-factor.

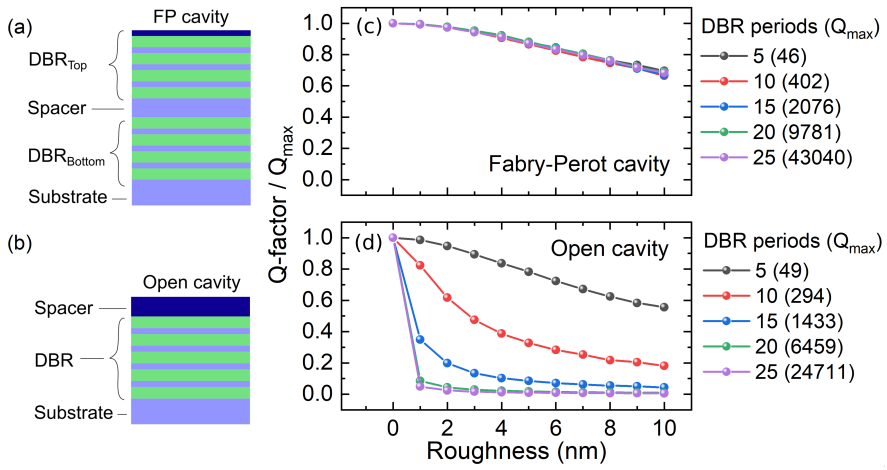

Figure 1. (a,b) Schematics of (a) Fabry- Perot resonator with a 16-period top DBR and a 20-period bottom DBR and (b) open cavity with 20 DBR periods and $\lambda/2$ spacer. (c,d) Effects of roughness on the Q-factor of (c) a $\lambda/2$ cavity Fabry-Perot resonator, and (d) a $3\lambda/2$ open-cavity resonator for various DBR configurations. In both panels, the bottom DBR varies from 5 to 25 bilayers in intervals of 5, while in (c) the top DBR of the Fabry-Perot comprises 4 bilayers less than the bottom one in all cases.

For structures with flat surfaces ($\sigma = 0$ nm), the Q-factor is solely determined by the number of DBR periods. However, as surface roughness increases, the effectiveness of stacking additional layers significantly wanes. This is

due to the upper Q-factor limit imposed by increased fluctuations in resonant frequencies, introduced by surface roughness. Although negligible for applications where ultrahigh Q-factors are not a requirement, this effect might have drastic consequences in specific applications, such as polaritonics and single photon sources .[2,3] This effect is considerably more prominent in open-cavity resonators than in Fabry-Perot ones, as depicted in Figure 1. In essence, higher roughness dictates a reduced number of DBR periods required to attain the maximum Q-factor in the structure, consequently leading to diminished maximum Q-factor values.

For instance, an open resonator composed of GaAs-with its characteristic low roughness (approximately one monolayer)-would benefit from an increased number of DBRs. Specifically, assuming a 0-nm-roughness GaAs/AlAs acoustic Bragg mirror consisting of 20 periods achieves a Q-factor of 6459, while 25 periods a Q-factor of 24711, and continually rising as more layers are added. Conversely, 1-nm-roughness would result in a Q-factor of 476 for 20 DBR layers and 505 for 25 DBR layers or more (Q-factor saturates above 25 layers), demonstrating a significant reduction of the Q-factor even for such minor roughness. Additionally, when the same resonator possesses a 2 nm roughness on its top layer, or a material with this roughness is deposited on top of it, the Q-factor saturates already at 20 DBR layers and adding more layers fails to increase it, as indicated in Fig. 1(d).

A comparison between the FP and open cavity configurations, reveals that the open cavity Q-factor is more sensitive to surface roughness than the FP cavity. Notably, even under relatively high surface roughness conditions (10 nm), the Q-factor of the FP cavity does not saturate; although it decreases to approximately 50 % of its maximum value. Overall, our study suggests that factoring in roughness becomes imperative when engineering high-quality photonic or acoustic resonators. Doing so, would enable precise Q-factor evaluations for each design, and prevent superfluous layer stacking. This, in turn, would improve device design, enhance operational efficiency, and minimize costs. When working with acoustic resonators at higher frequencies, and hence thinner layers, the effect of roughness is extremely critical.

Regarding the DBR unit cell layers' thicknesses, Fig. 1 presents results for $\lambda/4 - 3\lambda/4$ (with respect to the acoustic wavelength λ). It is worth noting that analogous conclusions hold for $\lambda/4 - \lambda/4$ DBRs. Since the overarching findings remain similar, we present here detailed results solely for the former case. We note two differences when the $\lambda/4 - \lambda/4$ unit cell is used; first, the stop band becomes twice broader, and second, the mode's resonant frequency exhibits an increased dependency on the top layer inhomogeneity.

4. DISCUSION AND CONCLUSIONS

In this study, we conducted an analysis of the impact of top layer thickness inhomogeneities on the quality factor and performance of acoustic and optical resonators based on GaAs/AlAs DBRs. Our findings reveal that thickness inaccuracies appreciably influence the mode frequency, while even relatively small surface roughness, on the order of a few nanometers, significantly influences the quality factor. Consequently, these effects can have a substantial impact on the device performance of DBR microcavities. This important aspect is often overlooked in the design process, making it essential to consider surface roughness for optimal performance. Notably, our developed model allows us to determine the maximum achievable quality factor and the minimum number of DBR layers required to achieve it, for different surface roughness values. By doing so, we can eliminate the need for growing unnecessary additional layers that do not contribute effectively, leading to more efficient and cost-effective designs.

We observed that surface thickness inhomogeneities affects acoustic cavities more prominently than their optical counterparts, although both are influenced. Additionally, open-cavity designs are much more sensitive to roughness compared to FP cavities, which is expected due to the closer proximity of roughness to the cavity region, leading to a more pronounced interaction. We believe that the insights obtained in this study have broad implications for the design of efficient optoelectronic, photonic, and acoustic devices.

5. ACKNOWLEDGEMENT

The authors acknowledge funding from European Research Council Consolidator Grant No.101045089 (T-Recs). This work was supported by the European Commission in the form of the H2020 FET Proactive project No. 824140 (TOCHA).

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