# Optical Bound States of 2D High-Contrast Grating for Refractometric Sensing

Yifei Wang<sup>1</sup>, Liang Dong<sup>1,\*</sup>, and Meng Lu<sup>1,2,\*</sup>

<sup>1</sup>Department of Electrical and Computer Engineering, Iowa State University, Ames, IA 50011 <sup>2</sup>Department of Mechanical Engineering, Iowa State University, Ames, IA 50011 \*email: Idong@iastate.edu and menglu@iastate.edu

**Abstract:** We report the numerical study of optical bound states in the radiation continuum using a silicon-based 2D high-contrast grating. The results show two distinct bound states at 1549.2 nm and 1743.1 nm. The high-Q resonances present near the bound states are exploited as a label-free biosensor.

OCIS codes: (230.0230) Optical device; (140.4780) Optical resonator; (280.1415) Biological sensing and sensors

## 1. Introduction

High contrast grating (HCG) is a planar subwavelength grating structure, where the grating material has a greater refractive index than its surrounding materials [1]. The HCG structure can be designed to exhibit three different types of optical responses: broadband high reflectivity, broadband high transmission, and high-Q Fano resonance [2]. Recently, Yoon *et al.* numerically studied the bound states in the continuum using a 1D periodic silicon grating [3]. A similar bound state was experimentally demonstrated by Hsu *et al.* using a Si<sub>3</sub>N<sub>4</sub> photonic crystal slab [4]. Here, we numerically investigate the bound states of two-dimensional (2D) silicon HCG structures made on a silicon-on-insulator (SOI) substrate. Two bound states in the radiation continuum are identified at 1549.2 nm and 1743.1 nm. Both of the bound states show a zero tangential wave vector ( $\mathbf{k}_{1/2} = 0$ ) and transit to high-Q resonance modes with Q-factors over 10<sup>5</sup> when  $\mathbf{k}_{1/2}2\pi < \pm 0.001$ , where *a* is the period of the lattice. The present HCG device has a high index sensitivity of 368 nm/RIU (refractive index unit), thus showing promises to explore refractive index-based sensing.



Figure 1. (a) Schematic of the 2D HCG structure and (b) SEM image of fabricated silicon nanoposts (Scale bar: 2 µm).

### 2. Optical bound states of 2D HCG

The HCG structure was designed for the bound states in the near-infrared region using a SOI substrate with a 500 nmthick silicon device layer (figure 1(a)). Figure 2(b) shows the scanning electron microscopic (SEM) image for a 2D array of silicon nanoposts fabricated using electron-beam lithography and reactive ion etching. The period, grating height, and post diameter of the HCG device is  $\Lambda = 1000$  nm,  $t_{Si} = 500$  nm, and d = 570 nm, respectively.



Figure 2. (a) Dispersion diagram of the HCG device. (b) Reflection spectra for several angles of incidence for region I (top) and region II (bottom). (c) Near field distributions of high-Q resonances at 1546.54 nm (top) and 1742.85 nm (bottom) when  $\theta = 0.5^{\circ}$ .

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Rigorous coupled-wave analysis was used to calculate reflection spectra and near field distributions associated with the resonant modes. Figure 2(a) shows the calculated spectral reflectivity for linearly polarized light with the angle of incidence ( $\theta$ ) ranging from -15 ° to 15 °. When  $\theta = 0$  °, there are two distinct bound states locating at 1549.2 nm (region I) and 1743.1 nm (region II), respectively. At the bound states, the Q-factor approaches infinite without considering the effect of material losses. A slight increase of  $\theta$  results in HCG resonances with finite Q-factors as illustrated in figure 2(b). The HCG resonances in region I exhibit strong and narrowband reflectance. In contrast, the modes in region II are associated with nearly zero reflectance at the resonance wavelength. In addition, the Q-factor can be tuned by adjusting the angle of incidence. Figure 2(c) presents the calculated near field distributions within one period of the HCG structure for two resonance modes at  $\lambda = 1549.2$  nm (top) and at  $\lambda = 1743.1$  nm (bottom).

The spectral signature of 2D HCG structure is also sensitive to geometric parameters, such as  $\Lambda$ ,  $t_{Si}$ , and d. These parameters can be well controlled to achieve the desired HCG resonance. For example, figure 3(a) and 3(b) show the spectral reflectivity as a function of duty cycle ( $d/\Lambda$ ) and grating height at  $\theta = 0.2$  °. As circled in figure 3, the high-Q HCG resonances are always present in the wavelength of 1450 nm to 1800 nm.



Figure 3. (a) Reflection spectra as a function of duty cycle. (b) Reflection spectra as a function of grating depth.

## 3. Refractometric sensing

The high-Q modes near the bound state (region I) are exploited for the development of refractive index-based labelfree biosensor. Compared to the existing high-Q optical biosensors [5], the resonance modes of 2D HCG device can be easily excited via surface-normal coupling, and more importantly, they exhibit high index sensitivities. Figure 4(a) shows the reflection spectra of HCG device when its surface is immersed in solutions with the refractive index ranging from 1.31 to 1.40 and  $\theta = 0.1^{\circ}$ . The bulk refractive index sensitivity can be calculated as  $S_b = \Delta \lambda / \Delta n = 368$  nm/RIU. The surface shift sensitivity is simulated by adding a monolayer of polymer material or protein (n = 1.45 and thickness of 15 nm) on the sidewall of the silicon nanoposts. Figure 4(b) compares the reflection spectra of the bare and the protein coated HCG devices. Owing to the monolayer coating, the resonant wavelength shifts approximately 2.7 nm.



Figure 4. (a) Simulated reflection spectra when HCG surface is immersed in solution with 10 different refraction indices. (b) The reflection spectrum while a thin layer of protein added.

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