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Gas sensing using a resilient polymer photonic crystal nanocavity with ultra-high quality factor

Hannah Clevenson¹, Pierre Desjardins², Xuetao Gan², Dirk Englund¹

¹Dept. of Electrical Engineering and Computer Science, Research Laboratory of Electronics, Massachusetts Institute of Technology, 77 Massachusetts Ave, Building 36-597. Cambridge, MA 02139, USA

²Dept. of Applied Physics, Columbia University, 530 West 120th Street, New York, NY 10027, USA hannahac@mit.edu

Abstract: We present a high-sensitivity, multi-use optical gas sensor based on a onedimensional polymer photonic crystal cavity. With an experimental Q exceeding 13100, we predict detection levels on the parts-per-billion range for a variety of gases.

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1. Introduction

Sensing volatile gases and alcoholic vapors is very important in a variety of fields, from law enforcement and national security to industrial and environmental safety. There are many advantages to using optical sensors for these applications, including high signal-to-noise ratio, high resolution of detection, operation in ambient conditions, electromagnetic immunity and electrical isolation, physical compactness and lightness, and a wide dynamic range. Photonic crystal cavities and resonators are able to further amplify these optical signals. Previous work has used materials that are sensitive to particular vapors, such as polymers, as coatings for their optical sensors [1–3]. We construct our sensor out of these sensitive polymeric materials, yielding increased sensitivity and resolution.



Fig. 1. a) Side view of the electric field $(|E|^2)$ of the fundamental mode in the 1D ladder nanobeam cavity. For a lattice constant *a*, the width w = 2.8a, d=1.4 a, $h_x = 0.52a$ and $h_y = 0.84w$ b) Top view of the same structure, c) Profile of the field, d) An SEM micrograph of the fabricated structure, and e) optical image of device. Note for d) and e) 1D device dimensions are 810 nm by 9.10 um.

Poly(methyl methacrylate) (PMMA) is an inexpensive, flexible, versatile, resilient polymer that swells in the presence of isopropyl alcohol (IPA) vapor, as well as several other gases, including ethanol. Additionally, PMMA is an electron beam lithography (EBL) resist, making the device simple to fabricate, as it requires no extra wet or dry etching steps. However, due to the low refractive index of PMMA and other polymer materials, total internal reflection is difficult to achieve when clad in another material. To overcome this challenge, we developed suspended structures, or "air-clad" devices, creating a sufficient change in refractive index. Figures 1a, 1b, and 1c show the fields inside our one-dimensional quadratically-tapered photonic crystal cavity design and 1d is an SEM micrograph of a fabricated device.

2. Theory

We assume that the polymer photonic crystal expands volumetrically with a change in volume, ΔV . This expansion occurs proportionally to the concentration of the stimulant gas in the system, until some saturation point. In the initial linear region, we describe this as: $\frac{\Delta V}{V} = c_o C$, where c_o is a constant and *C* is the concentration of the gas. Next, we describe strain in terms of the gas concentration. Strain is defined as $\varepsilon = \frac{\Delta L}{L}$, where L is the length of the structure. This is roughly equivalent to $\frac{\Delta V}{V}$ for a one-dimensional structure, yielding: $\varepsilon = \frac{\Delta V}{V} = c_o C$. This is also proportional to $\frac{\Delta \lambda}{\lambda}$ by some constant c_1 . We describe the linewidth of the spectral peak to be as follows: $\sigma_{\lambda} = \frac{\lambda}{Q} \cdot \frac{1}{\sqrt{T \cdot \tau}}$ where *Q* is the quality factor, λ is the center wavelength, *T* is the intensity (counts/s), and τ is the integration time. The minimum detectable concentration occurs when the change in wavelength, $\Delta \lambda$, is equal to the width of the spectral peak, σ_{λ} . This gives us a minimum detectable strain of $\varepsilon = \frac{c_1}{Q} \cdot \frac{1}{\sqrt{T \cdot \tau}}$ and a minimum detectable concentration of $C = \frac{c_1}{c_o \cdot Q} \cdot \frac{1}{\sqrt{T \cdot \tau}}$. Experimentally, we have found *Q* values up to 13130, $T \approx 1000$ counts/s, and $c_1 \approx 1$. We estimate $c_o \approx 5x10^{-4}$ as in [3]. This gives an estimate of the concentration sensitivity $S = \frac{c_1}{c_o \cdot Q} \cdot \frac{1}{\sqrt{T}} = 5 \ ppb/\sqrt{Hz}$.

3. Experimental

We spin-coat a 10 *nm* thick layer of water-soluble polyvinyl alcohol onto a silicon substrate, followed by 400 *nm* of PMMA (doped with Coumarin 6 dye, 5% by weight). The patterns are defined using EBL, then immersed in water, allowing the PMMA film to float to the surface, where it can be transferred to any rough or patterned carrier, including spun fiber tissue paper (Fig. 1e). The devices are tested on a confocal microscope setup with independent pump and collection paths. The stimulant gas concentration in the system is controlled by a dilution gas flow setup.



Fig. 2. a) Polymer cavity with peak at 627 nm and Q = 13134. b) Initial tests showing the recovery of the device after the stimulant is removed, with respect to resonant wavelength. Note that some bleaching of the dye does occur – this can be remedied by using input and output coupler gratings with an external light source instead of the dye as an internal light source.

4. Discussion

Initial tests analyzed IPA vapor, though any gas or vapor that interacts with the polymer film can be used. The device is exposed to 15 sccm dilute gas flow (1:60 equilibrium vapor pressure IPA:air, $\sim 600 \ ppm$) for 5 minutes, then exposed to pure air flow for 20 minute for recovery. We show high Q cavities (Fig. 2a) and full recovery of the sensor after the IPA vapor has been removed from the system (Fig. 2b). Additionally, low concentrations of destructive vapors can also be detected, such as ozone and acetone vapor.

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