Photonic Crystal Nanocavity with Atomically Flat Si (111) Interfaces

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Photonic crystals (PhC) nanocavities possess many intriguing properties, which are useful to investigate fundamental light-matter interactions as well as the applications to various silicon (Si) photonics devices. However, their characteristics are very sensitive to structural disturbances induced during fabrication, which makes the production of such structures still a practical challenge for mass production. Current fabrication processes, such as optical lithography combined with dry etching, often result in unavoidable line-edge roughness on the sidewalls. This leads to scattering losses inside cavities, hence posing a limit to the strength of light confinement. To mitigate the fabrication-induced losses inside nanocavities, we propose to use atomically flat Si (111) planes that can be fabricated through anisotropic wet etching. Si (111) planes have a much slower etching rate in alkali wet etchants compared to other planes, thus capable of producing atomically flat interfaces with reduced roughness. In addition, the etching is self-limited, which means the manufacturing tolerance against processing can be expanded, while we must accommodate the design limitations of using the flat planes.

In this paper, we theoretically have examined the impacts of Si (111) surfaces on the optical confinement capabilities of 2-dimensional PhC nanocavities. We assumed a 300-nm-thick Silicon-On-Insulator (SOI) substrate with the Si (110) surface on the top SOI layer. Employing anisotropic wet etching on the top layer allows us to define surfaces perpendicular to the substrate in the <110> and <112> direction. These surfaces will form lattice points in the shape of parallelograms with interior angles of 70.53° and 109.47°. Utilizing this uniquely shaped lattice point, a variety of lattice configurations were constructed and their their photonic band gap properties were determined through simulations using the plane wave expansion method. Based on the band gap results, we introduced H0-, H1- and L3-nanocavities into each structure and optimized the lattice period a and the width of the lattice point l to localize a light of wavelength 1550 nm exactly in the center of the band gap. The H0 cavity was formed by shifting two adjacent lattice points in the center outward in the x-direction by $0.12a$. The H1 and L3 cavities were formed by removing one and three adjacent lattice points from the center of the lattice respectively. We computed the quality factor Q and the modal volume V using the finite-difference time-domain approach in the transverse electric (TE) mode. To describe the strength of the optical confinement, the ratio of Q/V, which is proportional to the Purcell factor, is used. The results show that a Q value of approximately 7,000 would be achievable. With Q/V values in the range of 10^3-10^4 λ^{-3}, these nanocavities will offer relatively strong confinement with huge manufacturing tolerances.

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