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Light propagation in planar optical waveguides made of silicon nanocrystals buried in silica glass

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Abstract

Silicon nanocrystals fabricated by Si⁺-ion implantation (400 keV, fluences from 4 to 6×10^{17} cm⁻²) of fused silica form interesting active planar optical waveguides. The nanocrystals emit orange-red photoluminescence (PL) (under UV-blue excitation) and define a region of high refractive index that guides part of the PL along the layer. Light from external light sources can also be coupled into the waveguides (directly to the polished edge facet or from the surface by applying a quartz prism coupler). In both cases the optical emission from the sample facet exhibits narrow (10–20 nm full-with-at-half-maximum) polarisation-resolved transverse electric and transverse magnetic modes instead of the usual broad nanocrystal spectra. This effect is explained by our theoretical model, which identifies the microcavity-like peaks as leaky modes propagating along the waveguide/substrate boundary (not the usual modes guided inside the nanocrystal plane due to its graded index profile). The unconventional properties of this relatively easy-to-make all-silicon structure may be interesting for future photonic devices and sensors. © 2005 Elsevier B.V. All rights reserved.

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1. Introduction

Research in silicon-based photonics aims to create integrated electronic and photonic functionality in a single silicon chip. Silicon nanocrystals (Si-NCs) are an important building block for such photonic circuits as they are efficient light emitters [1] and their assembles can be used to form active optical waveguides [2]. For example, it was recently shown that Si-NC waveguides, with properly designed refractive index profile, exhibit spectral filtering and pronounced polarization of the Si-NC photoluminescence (PL) emission [3,4]. This unexpected effect was shown by our group to be due to leaky modes of the lossy planar waveguides [5]. In this paper we compare the propagation of PL excited inside the waveguide with that of light coupled from external sources.

2. Sample preparation and experimental techniques

The Si-NC waveguides were prepared by 400 keV Si⁺-ion implantation into optically polished Infrasil slabs with fluences of 4.0, 4.5, 5.0, 5.5, and 6.0×10^{17} cm⁻². Samples were subsequently annealed for 1 h at 1100 °C in a N₂ ambient to form Si-NCs and further annealed for 1 h at 500 °C in forming gas (N_2/H_2) to enhance the PL. The diameter of Si-NCs was estimated from Raman scattering spectra to be about 5 nm [6]. The implanted layer buried in a silica slab acts as a planar asymmetrical optical waveguide. Refraction index profiles were estimated from SRIM (the Stopping and Range of Ions in Matter [7]) calculations of implantation profiles and from modelling of VIS-IR transmission fringes [5] (the peak refraction index increases from 1.75 to 2 with increasing implantation dose). The profiles are asymmetric Gaussians with a peak around 600 nm below surface and a full-width at half-maximum of about 300 nm.

Photoluminescence was measured at room temperature under excitation with an Ar-ion laser (458 nm) or He-Cd

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Fig. 1. Schematics of experimental set-ups: (A) PL measurements, (B) external source coupling through a prism (a) or directly through the facet (b).

laser (325 or 442 nm) and detected with an imaging spectrograph (Jobin–Yvon Triax 320) coupled to an i-CCD camera (Princeton Instruments PI-MAX). All spectra were corrected for the experimental system response. Light coming from the sample was collected by a quartz fibre (mounted on a goniometer) and imaged on the spectrograph input, the collection angle being of about 1° (see Fig. 1A). For comparison we coupled external light sources (Xe lamp, halogen lamp or white LED) to the waveguide either through a quartz prism or directly through the polished edge of the sample (arrows *a* and *b*, respectively, in Fig. 1B). A black shield and a prism on the bottom of the sample eliminated direct detection of light and reflections from the sample interface, respectively.

3. Experimental results

PL measurement of the samples under UV excitation at about 45° and with signal collection perpendicular to the layer shows a wide PL band centred around 850 nm which is almost equal for all implantation fluences (upper spectra in Fig. 2A). Such broad-band spectra are typical of the inhomogeneously broadened emission from Si-NCs. In contrast, the PL spectra collected from the edge of the sample or for angles of a few degrees below the plane of the waveguide ($\alpha > 0$ in Fig. 1), reveal pronounced spectral filtering and polarization. The "facet" spectra are composed of two distinct peaks separated by about 30 nm, which are systematically red-shifted with increasing implantation fluence (lower spectra in Fig. 2A). The short-wavelength peak has linear polarization parallel to the Si-NCs layer (TE-polarization) while the long-wavelength one has polarization perpendicular to the film (TM-polarization) (see Fig. 2B).

The external-light coupling experiments using a quartz prism show the best transmission in the "facet" direction or slightly below ($\alpha \sim 7^{\circ}$). The transmission spectra consist of two broad bands (Fig. 3A) with a small degree of polarization. The spectral positions of the long-wavelength bands agree with the luminescence TE and TM peaks of respective layers. The coupling of light directly through the polished facet is more delicate but is also possible. Fig. 3B compares the two coupling methods for the sample implanted with fluence of 5.5×10^{17}

 $\rm cm^{-2}$. The direct coupling gives much narrower absorption peaks with distinct TE and TM resolution.

4. Discussion of the guiding mechanism

Two different mechanisms were proposed to explain this novel guiding behaviour:

(i) The linearly polarized PL peaks could simply result from standard guided modes of the planar waveguide. However, an ideal transparent planar waveguide should transmit a continuous spectrum of guided modes up to a cut-off wavelength [8], which is estimated to lie above \sim 1500 nm for the first order modes in our waveguides. Some spectral structure might arise from wavelength dependent losses, with those modes (wavelengths) that undergo the smallest loss being guided to the edge of the sample. These are likely those modes that are "weakly guided", i.e. the modes whose electric field is strongly delocalized and the modes that propagate basically as a planar wave in the substrate [3,8]. Their effective guide thickness approaches infinity. Ray optics describes these modes by an angle of incidence θ that is *greater than* but very close to the critical angle θ_{c} for total internal refection. The salient feature of the filtering, namely, the



Fig. 2. (A) PL spectra of layers implanted with fluences of 4 to 6×10^{17} cm⁻². The upper spectra are taken perpendicular to the plane of waveguide layer, while the lower spectra are taken from the facet at angle of 7°. The TE/TM peaks shift to longer wavelength with increasing implantation fluence. (Note the log scale of PL intensity). (B) Polarization resolved PL spectra of the sample 5.5×10^{17} cm⁻² taken for angle 7°. TE and TM peaks (black dots and open squares, respectively) are linearly polarized parallel or perpendicular to the implanted layer, respectively.



Fig. 3. (A) Transmission spectra for white light coupled to the waveguides through the quartz prism placed on the upper surface of waveguide. Detection angle was 7° . The two spectral bands are systematically red-shifted with increasing implantation fluence. (B) Comparison of short-wavelegth transmission peak for prism-coupling (a) and transmission dip for direct coupling through the facet (b). The TE and TM polarizations are represented by dash and dot-dash lines, respectively.

separation between TE and TM modes, is a direct consequence of the asymmetric guide — different phase shifts Φ for the TE and TM modes under total reflection at both boundaries. In order to fulfill the phase condition that after two successive reflections the phase difference can only be equal to integral multiple of 2π , suitable wavelengths from the emission band are combined with available values of Φ . Since the latter are slightly different for TE and TM polarizations at a given angle of incidence, the resulting mode wavelengths are also slightly different.

(ii) The second possible mechanism involves substrate leaky (or radiation) modes of the Si-NCs waveguide [5,9]. These modes propagate at angle θ situated close to but *below* θ_c , undergo total reflection at the upper boundary Si-NCs/air (larger index difference) but are only partially reflected on the lower boundary Si-NCs/substrate (smaller index difference). Consequently, a small fraction of their power is radiated into the substrate at each bottom reflection. If the angle θ is only slightly less than θ_c , the leaky modes propagate nearly parallel to the Si-NCs plane. Moreover, the number of reflections is very high (reflectance is close to unity), resulting in a narrow spectral width of the modes. The mechanism of spectral filtering in this case remains basically the same as discussed above, the only difference being that a phase shift Φ at the upper boundary only comes in to play during the initial stages of propagation. After a finite number of internal reflections all the radiant power escapes into leaky modes and emerges from the sample facet in a well-defined direction, basically parallel to the Si-NCs film. This makes such leaky substrate modes virtually indistinguishable from the guided modes.

In our previous papers [5,6] we proved the validity of the leaky-mode model by numerical calculations and by experiment where drops of different liquids were placed on the surface above the excited spot or between the spot and the edge. In the first case the "facet" PL spectrum changes significantly depending on the refractive index of the liquid, while there are no changes with drops located some distance from the excited spot.

The prism-coupled transmission spectrum is broad with weak polarization dependence (Fig. 3A) because the number of reflections is very low and the waveguide becomes more symmetrical as the upper boundary is covered by the quartz prism (with an immersion oil). On the other hand, direct coupling through the facet reveals maxima of the absorption spectrum at the similar position as maxima of the transmission spectrum of the prism-coupled light. Properties of absorption spectra, namely, narrow spectral width and TE/TM splitting, are similar to the PL spectrum. However, in addition to one TE/ TM doublet in the red spectral region in PL there is another one in the blue-green region (Fig. 3B, b). These are likely modes of the third order (the red ones being second order and undetected first order lay in infrared region), which cannot be observed in PL experiments since there is no blue PL in our Si-NCs. We proved also that a liquid drop on the surface of the waveguide (see Fig. 1) has no significant influence on the detected spectrum in this case.

The attenuation of guided modes in our samples is attributed to waveguide losses. Surface and sidewall roughness is usually supposed to cause waveguide losses. But in our sample the measured RMS roughness is only about 0.5 nm [6]. The loss is therefore likely due to self-absorption and/or Mie scattering in the waveguide core and diffraction of the guided modes at the output facet. The shifted-excitation-spot (SES) measurements revealed losses for guided modes to be about 11 cm⁻¹ at 825 nm (implantation fluence of 4×10^{17} cm⁻²) [10].

5. Conclusions

We have demonstrated the principal role of substrate radiation modes (leaky modes) in the spectral filtration effect in thin-film Si-NCs waveguides. The special features of the leaky modes are: (i) directionality better than for conventional waveguides, (ii) a high degree of polarization, and (iii) certain spectral tunability via varying the preparation conditions. Such features are interesting for photonic devices and may be compared with the emission of Si-NCs in an optical microcavity [11,12] (without the need to fabricate Bragg reflectors). The consequences of this propagation mode for potential optical amplification (supposing the Si-NCs could give rise to stimulated emission) are being studied and will be published separately.

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