

Nanowire Geometry Engineering for Enhanced Fluorescence Biosensing Performance

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Summary:

We introduce a dual-function nanowire architecture consisting of a tapered tip integrated with a cylindrical base, enabling enhanced optical concentration while the cylindrical base preserves the imaging advantages of conventional nanowire biosensor. Our optics modelling shows that the proposed nanowire achieves $>1000\times$ fluorescence enhancement over planar substrates and outperforms a full-length cylindrical nanowire. We propose also an alternative nanowire geometry that eliminates the need for selective functionalization while retaining performance comparable to the top-tapered configuration.

Keywords: Nanowires, Biosensor, Fluorescence, Signal Enhancement, Imaging.

Background, Motivation and Objective

Optical biosensors are of great interest over electrochemical, electrical, or piezoelectric sensors because they offer exceptional sensitivity, allow label-free or fluorescence-based detection, and real-time monitoring [1]. Industry-standard planar fluorescence biosensors are popular for their simplicity and cost-effectiveness but are often limited by sensitivity and detection limits [2]. Nanowire (NW) biosensors are currently attracting significant attention because of their high surface-to-volume ratios and engineered geometries that enhance light-matter interaction and photon collection, enabling ultra-low-concentration biomolecule detection that surpasses conventional planar biosensors [3-4].

Recently, our group demonstrated through modelling that vertically oriented GaP NW achieved $>100\times$ fluorescence signal enhancement over planar biosensors and enabled imaging-based detection with 25-fold sharper images than conventional diffraction-limited microscopy [4].

The principal objective of this work is to advance fluorescence-based biosensing through the computational design and analysis of nanowire for enhanced signal and imaging performance. Accordingly, we propose a top-tapered nanowire with a cylindrical base to further enhance fluorescence signal and evaluate its imaging performance. The proposed nanowire achieves $>1000\times$ fluorescence enhancement compared with planar substrates and outperforms cylindrical nanowires in low numerical aperture (NA_{exc} and NA_{coll}) setups. These results are calculated assuming fluorophore binding only on the cylindrical region, which necessitates selective functionalization and may pose practical challenges. To address this, we also investigate an inverted-taper geometry that removes the need for

selective functionalization while preserving performance comparable to the top-tapered design.

Proposed Nanowire design

The nanowire consists of a cylindrical base that preserves the imaging performance of a non-tapered nanowire, combined with a tapered top section designed to enhance the optical signal (Fig. 1). Silicon (Si) is used as the nanowire material, compared to GaP, it is more cost-effective but exhibits some parasitic absorption, particularly at shorter visible wavelengths. We optimize for the operating wavelengths $\lambda_{exc} = 640$ nm and $\lambda_{em} = 670$ nm. The optical response is modeled using the finite element method in COMSOL Multiphysics. The cylindrical base length is fixed at $C_L = 1500$ nm, while the tapered length (T_L) is varied from 500 nm to 8500 nm.

To avoid selective functionalization, we also propose an inverted geometry (Fig. 2) where the nanowire tapered part is placed inside a lower refractive index substrate (e.g., $n \approx 1.5$). This configuration prohibits fluorophores from binding to the low-enhancement (tapered) region, removing the need for surface selectivity.

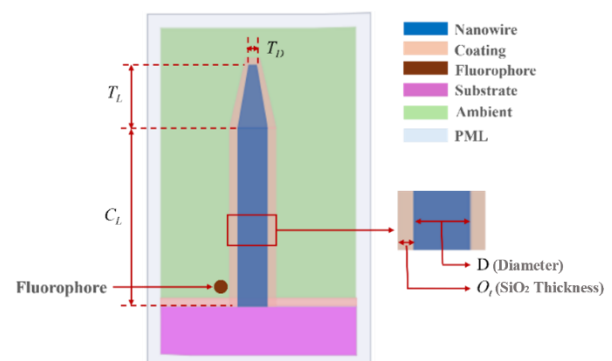


Fig. 1. Cross sectional view of the proposed top-tapered nanowire

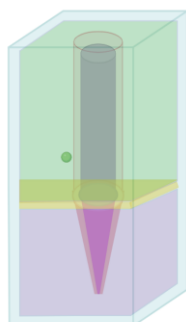


Fig. 2. 3D view of the proposed geometrical setup for avoiding selective functionalization.

Results

The proposed top-tapered NW provides more than three orders of magnitude higher fluorescence enhancement compared with the planar reference and approximately 10-fold improvement over the non-tapered configuration across all investigated fluorophore quantum yields under low NA. The enhancement continues further with taper length (Fig. 3). Fig. 3 also shows that the signal enhancement of the alternative inverted geometry, in which the tapered section is embedded in the substrate, achieves comparable performance while avoiding the need for selective functionalization. We further evaluate the imaging performance by analyzing the spatial localization of the collected signal around the nanowire position. Imaging is assessed from both top and bottom collection sides and presented in Fig. 4. For top-side imaging, $\langle \text{REL}_{\text{img}} \rangle$ decreases with increasing taper length due to the more directional emission induced by the taper. In contrast, for bottom-side imaging toward the cylindrical binding region, $\langle \text{REL}_{\text{img}} \rangle$ remains stable, with approximately 15% better image sharpness compared with a cylindrical nanowire. The inverted geometry also maintains comparable performance to the top-tapered design in both imaging configurations (Fig. 4).

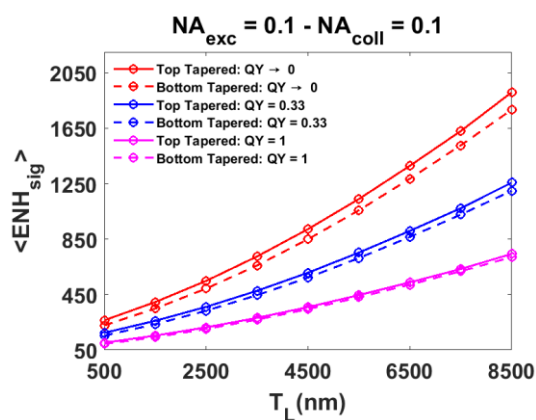


Fig. 3. Signal enhancement relative as a function of tapering length at low numerical aperture for both top and bottom tapered geometry.

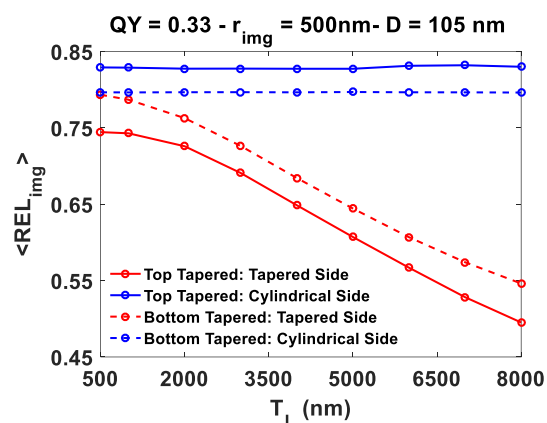


Fig. 4. $\langle \text{REL}_{\text{img}} \rangle$, the integrated counts in a disc of 500 nm in radius in the image plane, relative to all counts in the image plane for both top-tapered and bottom tapered situations and imaging from either top or bottom side.

Conclusion

Overall, the proposed nanowire architecture combines cylindrical and tapered geometries to achieve dual functionality. It enables strong fluorescence signal enhancement at low numerical aperture while maintaining stable imaging performance. In addition, the inverted configuration provides a practical route to eliminate the need for selective functionalization. This favorable low-NA performance supports improved signal strength and reliable imaging, making it well suited for cost-effective, compact, and easily integrable biosensing applications.

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