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Modelling and Design of a Microfluidic Platform for Precision Exposure to Environmental Samples of Surface-Enhanced Raman Scattering Sensors

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Summary:

SERS sensors offer high sensitivity for real-time molecular detection but face limitations due to sample drying and reproducibility in exposure to samples. Integrating SERS with microfluidics addresses these issues. Here, we discuss microfluidic designs and material selection to enhance SERS sensitivity and minimize background interference. Using Finite Element Method (FEM) simulations and experimental optical characterization, we systematically optimized designs for uniform SERS sensors exposure to liquid samples. The manufacturability of microfluidics in glass and wafer-level anodic bonding for integration were considered.

Keywords: Surface-enhanced Raman spectroscopy, microfluidics, water analysis, optical sensor

Background

Microfluidic SERS sensors are promising for real-time field monitoring of emerging contaminants in water, addressing public health, and climate change concerns (Fig.1) [1-3]. SERS excels in obtaining molecular "fingerprints" without labeling, detecting complex matrices, and being miniaturized for portable monitoring [4]. Sampling reliability and sensor-flow interaction are crucial [5]. Integrating SERS with microfluidics was shown to enhance detection [2,3].

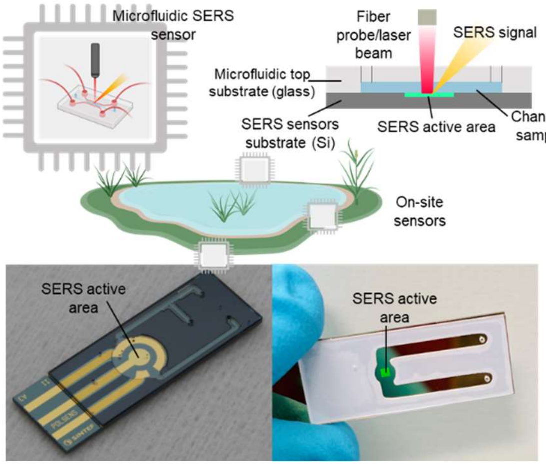

Fig. 1. Concept and examples of fabricated microfluidic SERS sensors [1-4] (part of the image is created with BioRender.com).

Reported microfluidic systems often lack a systematic approach to microfluidics design and material selection, as well as a manufacturability perspective. This publication addresses this gap.

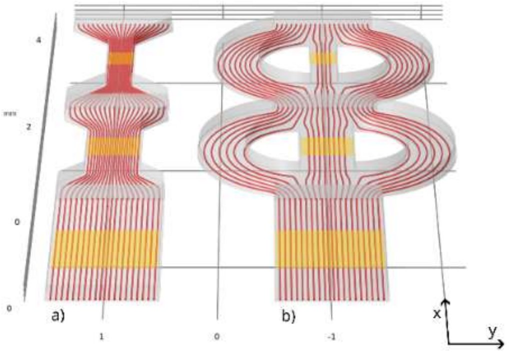

Fig. 2: Microfluidic channel designs, including flow lines, consisting of 3 consecutive SERS elements spaced by 2 mm. a) Tapered channel design, b) Side channel design. The location of the SERS areas is highlighted in yellow. The flow is along the x axis.

Description of the FEM model and aims

The main goal is to optimize the design of microfluidic channels to ensure uniform flow conditions across the entire SERS active area and at the interface with the liquid sample, preferring lower flow velocities that lead to longer interaction with the SERS surface. We aim at designs offering comparable performance for different SERS area sizes, which are combined within a single channel (Fig.2). We consider as baseline a channel with a cross-section of 1000x50 µm, optimizing the design while addressing

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technological and experimental issues. We aim for larger channel depths above SERS areas, as it has been experimentally observed that the optical detection through shallower channels can be compromised both due to high background reducing the SERS signal (Fig.3) and material properties generating additional Raman peaks (Fig.4). Considering the laser spot size of 84 µm, and need for alignment, it is desirable to have a channel not wider than the SERS area itself. With a straight channel design tapering to the SERS sizes, velocities would vary between designs and therefore require compensation. To address these issues, we consider two main additions to baseline design: 1) extra depth; 2) side channels, redirecting part of the flow from the SERS. The 3D model consists of a 2 mm long section of the channel, centered in the middle of the SERS area, which is also the middle of the channel. We model each design independently, to reduce computational load, assuming the flow returns to an unperturbed, fully formed creeping flow after each section. The model is symmetrical and solved for half the geometry (Fig.5a).

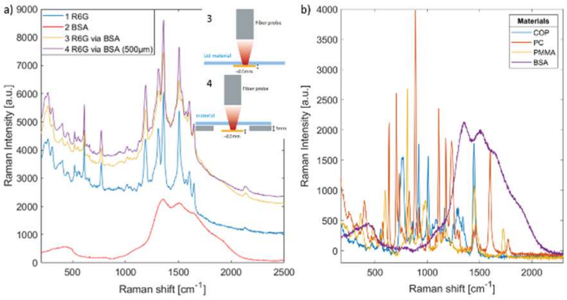

Fig. 3: Raman spectra of a) (1) Rhodamine 6G (R6G), (2) Borosilicate (BSA) fluidic substrate, (3) R6G measured via BSA in proximity, (4) R6G via BSA in a 0.5mm distance; b) Raman spectra of different microfluidic substrate materials

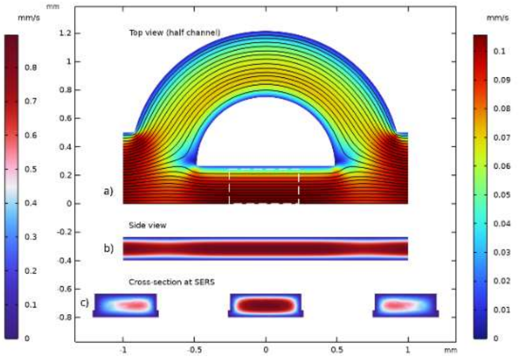

Fig. 5: Flow velocity norm for a proposed design with 500 µm SERS side length, 450 µm wide side channels, and extra channel depth. Velocities are uniform towards the center of the SERS area, inside the dashed line in a) and in the cross-section c).

Results and conclusions

Based on the FEM results (Fig.5, Table 1), while a 1 mm SERS area with extra depth† is the simplest and best performing design, cost and alignment issues suggest the need for a better solution. A 250 µm SERS area‡ could suffer from non-uniform and relatively larger flow velocities, affecting measurement quality. A 500 µm SERS area*, with extra channel depth and side channels, offers a good compromise between the two, with only 1/4 of the surface, flow velocities (v_{max}) comparable to the straight channel and relatively low transversal velocity falloff (δ_v^T).

Tab. 1: Main designs and flow characteristics.

SERS	Type	v_{max}	δ_v^T
1000	baseline	100%	0%
1000†	+depth	11%	0%
500	tapered, +depth	24%	2%
500*	side chan., +depth	12%	2%
250	tapered, +depth	56%	26%
250‡	side chan., +depth	14%	26%

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