

Supplementary Materials

Silica Nanospheres Coated Silver Islands as an Effective opto-plasmonic SERS Active Platform for Rapid and Sensitive Detection of Prostate Cancer Biomarkers

Anamika Pandey[†], Subhankar Sarkar[#], Sumit Kumar Pandey[†] and Anchal Srivastava^{†*}

[†]Department of Physics, Institute of Science, Banaras Hindu University, Varanasi-221005, India

[#]School of Computational and Integrative Sciences, Jawaharlal Nehru University, New Delhi-110067, India

*Corresponding author

Email: anchalbhu@gmail.com, anchal@bhu.ac.in

Ph.: +91-9453203122

Synthesis of SiO₂ nanospheres

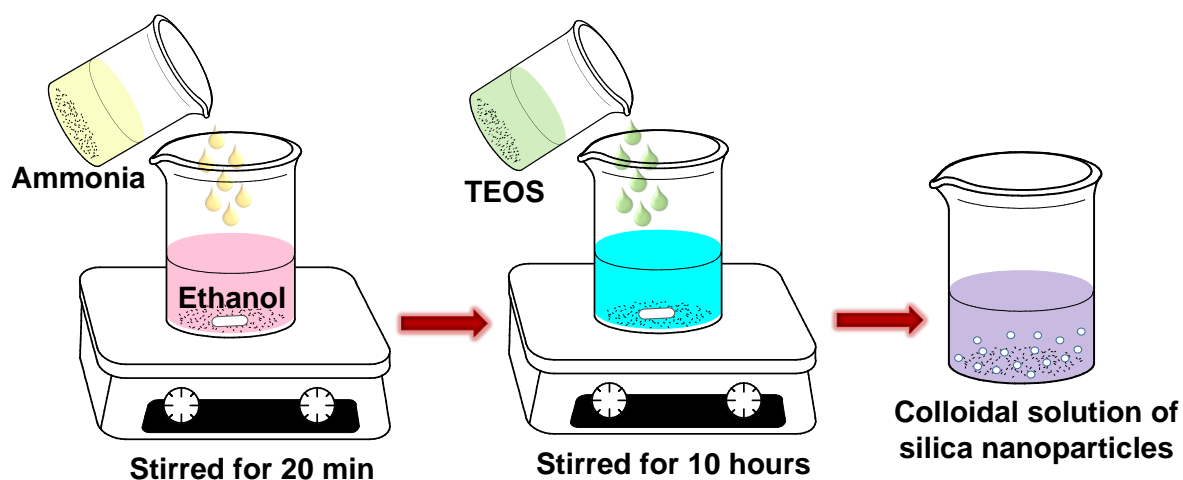


Figure S1: Schematic procedure for the synthesis of silica nanospheres *via* Stober's method.

Fabrication of SERS substrate

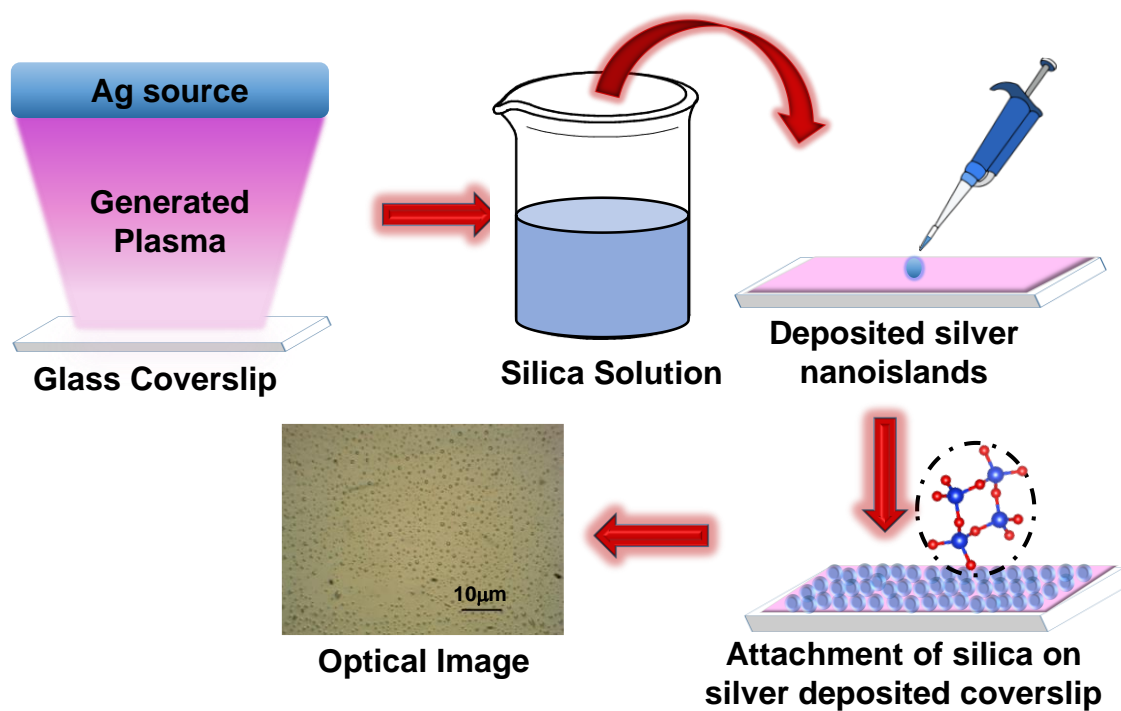


Figure S2: Schematic illustration of the fabrication of SERS substrate with the aid of RF sputtering.

SERS measurements

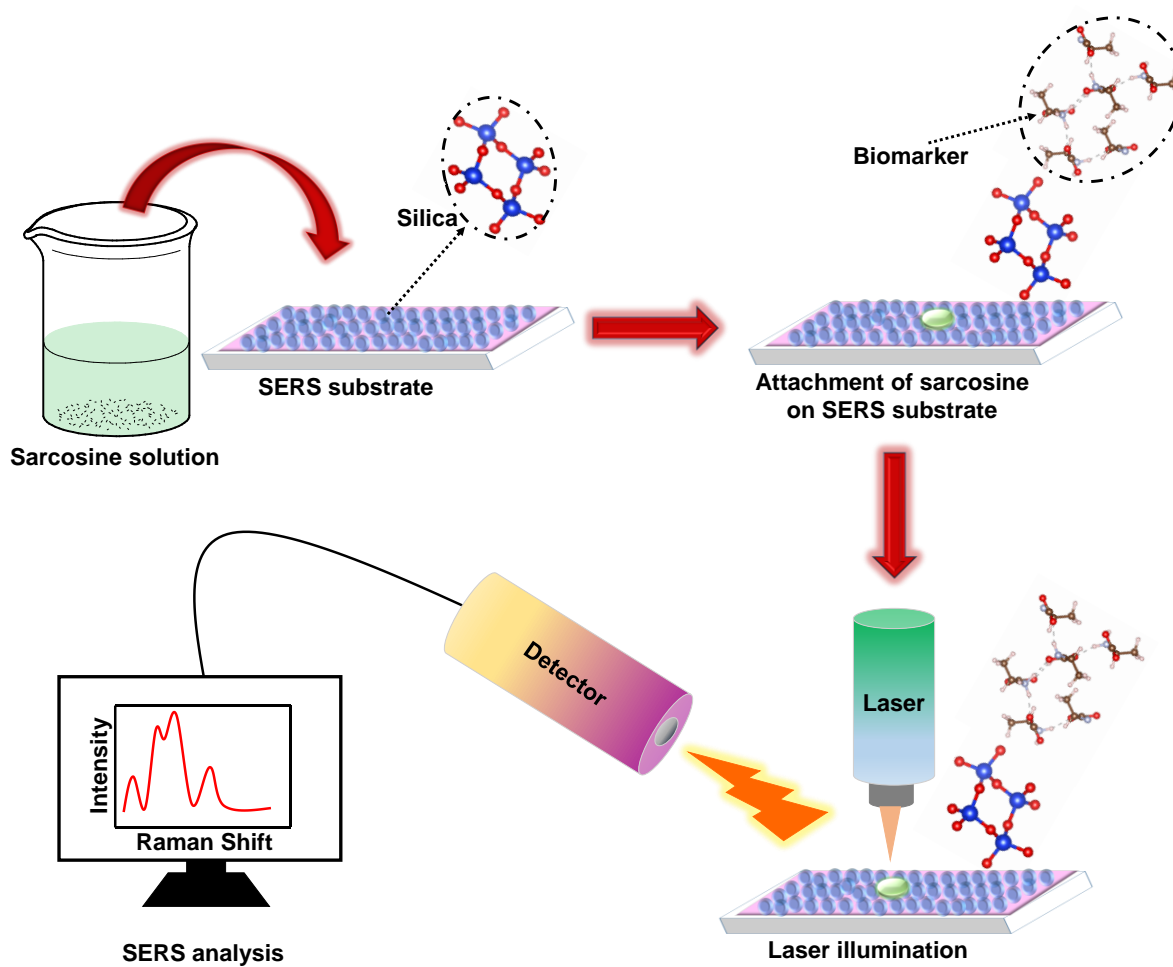


Figure S3: Schematic illustration of SERS analysis of sarcosine.

UV-vis absorption spectra of silica nanospheres and band gap calculation

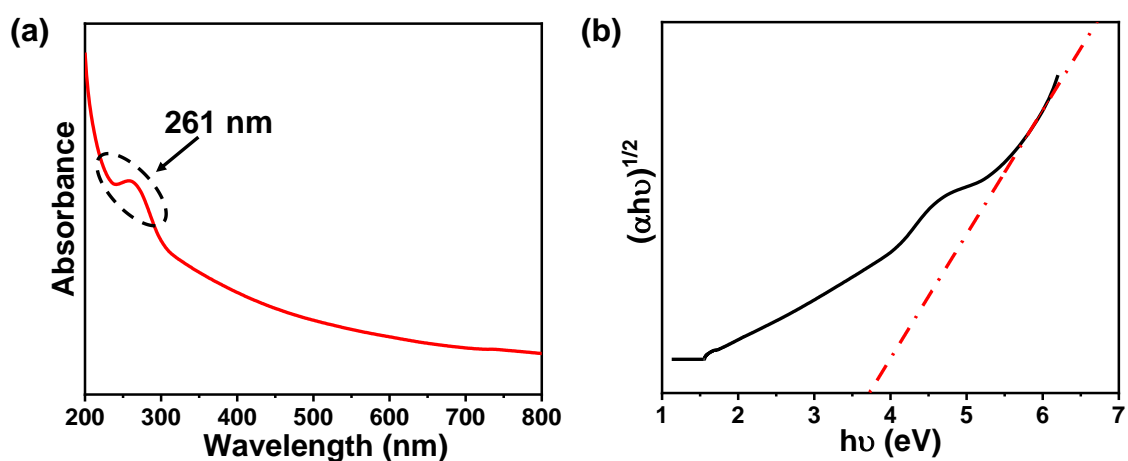


Figure S4: (a) UV-vis absorption spectra of as-synthesized SiO₂ nanospheres. (b) the band gap estimation of synthesized SiO₂ nanoparticles using Tauc's plot.

AFM 3D topography of silver nano-islands and silica nanospheres decorated silver nano-islands

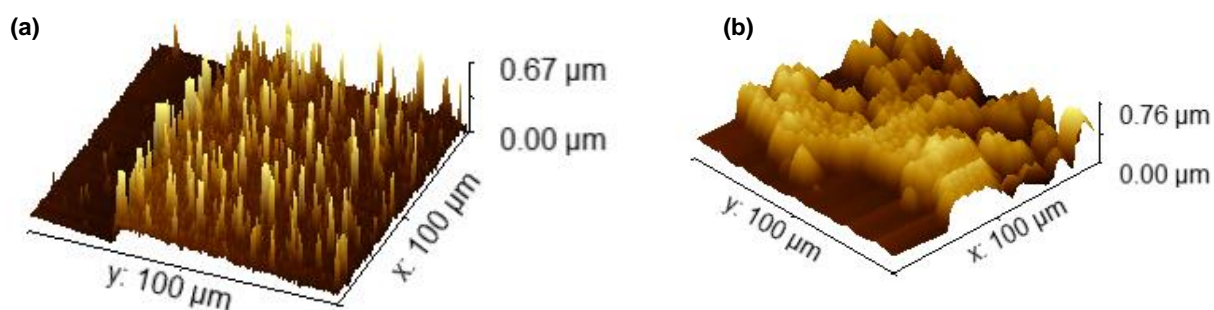


Figure S5: (a) 3D topography of silver nano-islands. (b) silica nanospheres decorated silver nano-islands.

Raman spectra of pure bulk sarcosine powder

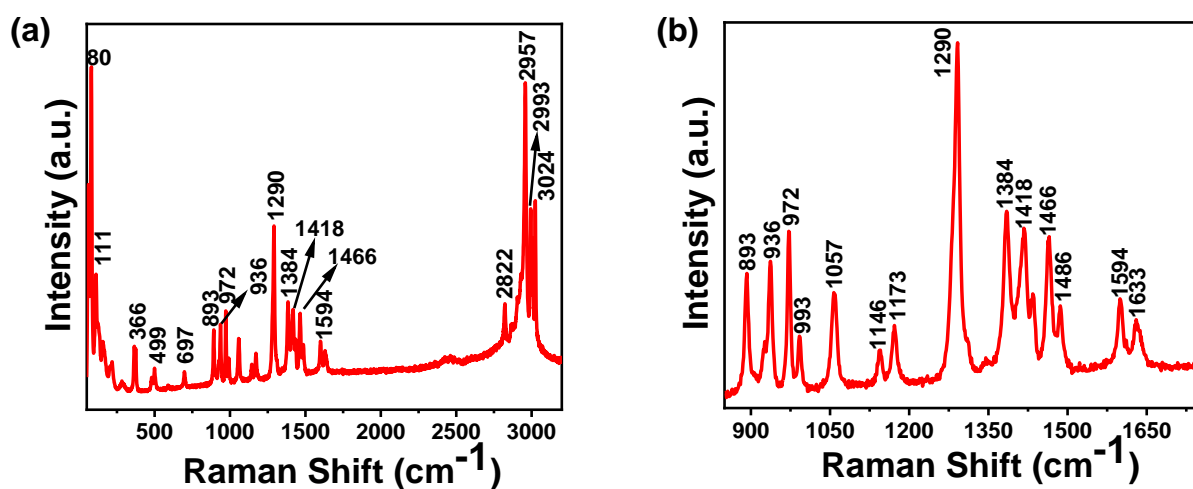
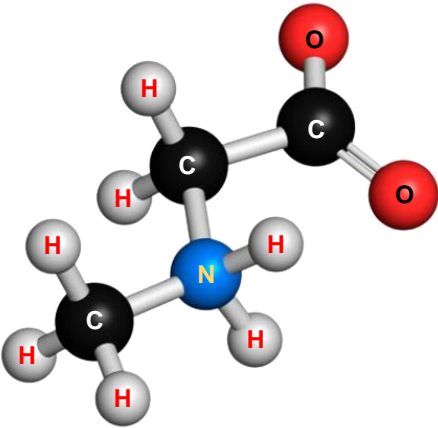


Figure S6: (a) Raman spectra of pure bulk sarcosine powder. (b) Raman spectra of pure bulk sarcosine powder within the range of 850 cm^{-1} to 1750 cm^{-1}

Table S1: The chemical structure and various vibrational Raman bands of the prostate cancer biomarker *viz* sarcosine.

Peak Position (cm^{-1})	Assignment	Relative Intensities (a.u.)
3024	CH_3 stretching (asymmetric)	8186
2993	CH_2 stretching (symmetric)	7919
2957	CH_2 stretching (symmetric)	12767
2822	CH_3 stretching (symmetric)	4191
1633	NH_2 deformation, $\text{C}=\text{O}$ stretching	2315
1594	COO^- stretching (asymmetric), NH_2 deformation	2674

	1486	CH ₂ rocking and deformation	2579
	1466	CH ₃ asymmetric in-plane bending, CH ₂ deformation	3771
	1418	COO ⁻ stretching (symmetric), CH ₂ deformation	3919
	1384	CH ₃ symmetric in-plane bending, CH ₂ deformation	4197
	1290	CC stretching	7166
	1173	NH ₂ rocking	2206
	1057	CO stretching	2803
	972	CH ₂ out-of-plane bending	3860
	936	COO ⁻ deformation, and CH ₂ rocking	3336
	893	CO stretching, CC stretching	3119
	697	COO ⁻ deformation	1536
	499	COO ⁻ rocking, C-N deformation	1671
	366	CH ₂ torsion	2495

Optical images of the SERS substrate before and after the Raman experiment

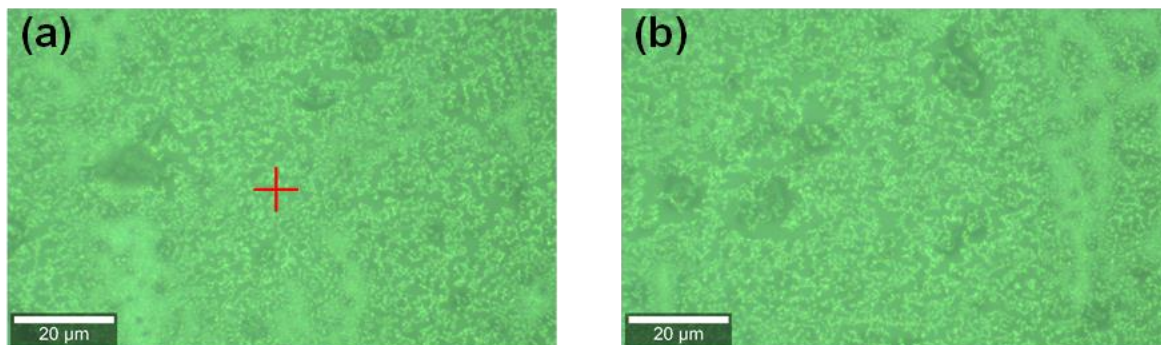


Figure S7: Optical images of SERS substrate (a) before Raman experiment (b) after Raman experiment.

Raman spectrum of prepared and used SiO₂@Ag SERS substrate

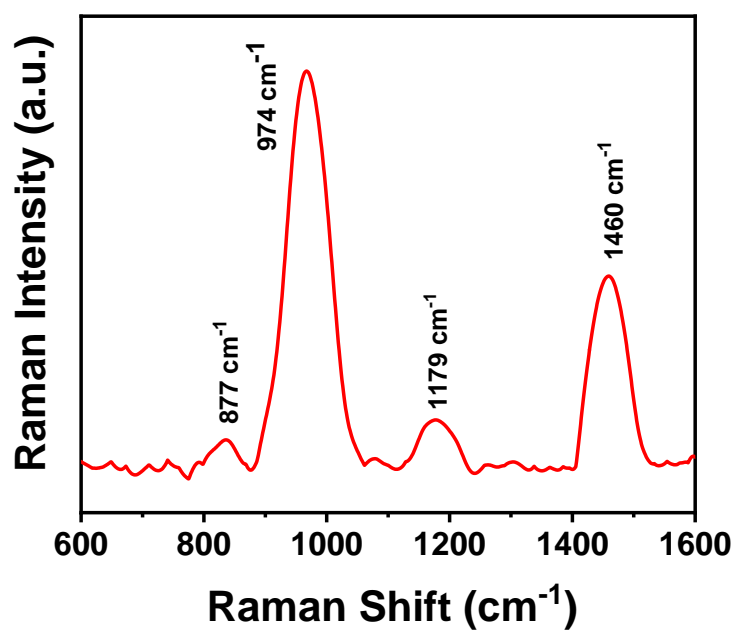


Figure S8: Raman spectrum of prepared and used SiO₂@Ag SERS substrate. The Raman spectrum shows peaks at 877 cm⁻¹ and 974 cm⁻¹ which corresponds to SiO₂ nanospheres. The peaks at 1179 cm⁻¹ and 1460 cm⁻¹ correspond to Ag nano-islands.

Calculation of limit of detection (LOD)

LOD of as fabricated SERS substrate has been calculated using the equation (1) given below

$$\text{LOD} = 3.3 \times (\text{SD of intercept/slope}) \quad (1)$$

SD (standard deviation) of intercept can be calculated by using the formula given below in equation (2):

$$\text{SD of intercept} = \text{SE (standard error) of intercept} \times \sqrt{N} \quad (2)$$

here, the value of SE of intercept is 9.847 which has been obtained using the calibration curve.

N is no. of the sample, i.e., 5. So, SD can be calculated as:

$$\begin{aligned} \text{SD of intercept} &= 9.847 \times \sqrt{5} \\ &= 22.017 \end{aligned}$$

From the calibration curve, the value of slope = 41.182

By substituting the values of SD of intercept and slope in equation (1), LOD can be calculated as:

$$\begin{aligned} \text{LOD} &= 3.3 \times (22.017/41.182) \\ &= 3.3 \times 0.534 \\ &= 1.76 \text{ nM} \end{aligned}$$

Hence, the LOD is found to be 1.76 nM.