

Supplementary Information for

Metal-Oxide Surface-Enhanced Raman Biosensor Template Towards Point-of-Care EGFR Detection and Cancer Diagnostics

Meysam Keshavarz¹, Panagiotis Kassanos¹, Bo Tan^{2,5}, and Krishnan Venkatakrishnan^{*,3,4,5}

¹ Hamlyn Centre for Robotic Surgery, Imperial College London, Bessemer Building, South Kensington Campus, Exhibition Rd, Kensington, London SW7 2AZ, UK

² Nanocharacterization Laboratory, Department of Aerospace Engineering, Ryerson University, 350 Victoria Street, Toronto, 5 Ontario M5B 2K3, Canada

³ Ultrashort Laser Nanomanufacturing Research Facility, Department of Mechanical and Industrial Engineering, Ryerson University, 9 350 Victoria Street, Toronto, ON M5B 2K3, Canada

⁴ Keenan Research Centre for Biomedical Science, St. Michael's Hospital, Toronto, Ontario M5B 1W8, Canada

⁵ NanoBioInterface facility, Department of Mechanical and Industrial Engineering, Ryerson University, 350 Victoria Street, Toronto, ON M5B 2K3, Canada

Email: venkat@ryerson.ca

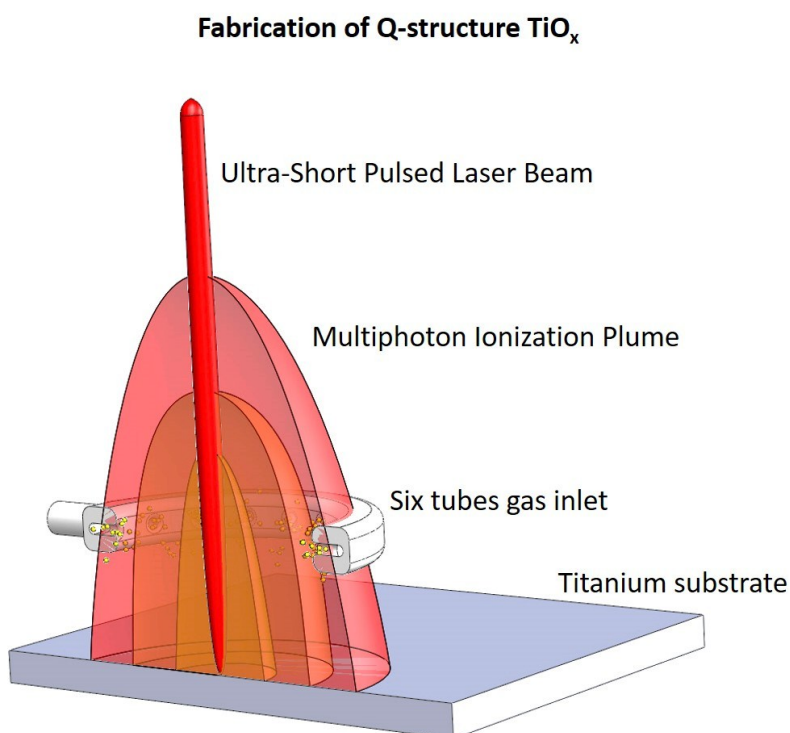


Fig. S1. Schematic illustration of fabrication of the Q-structured TiO_x.

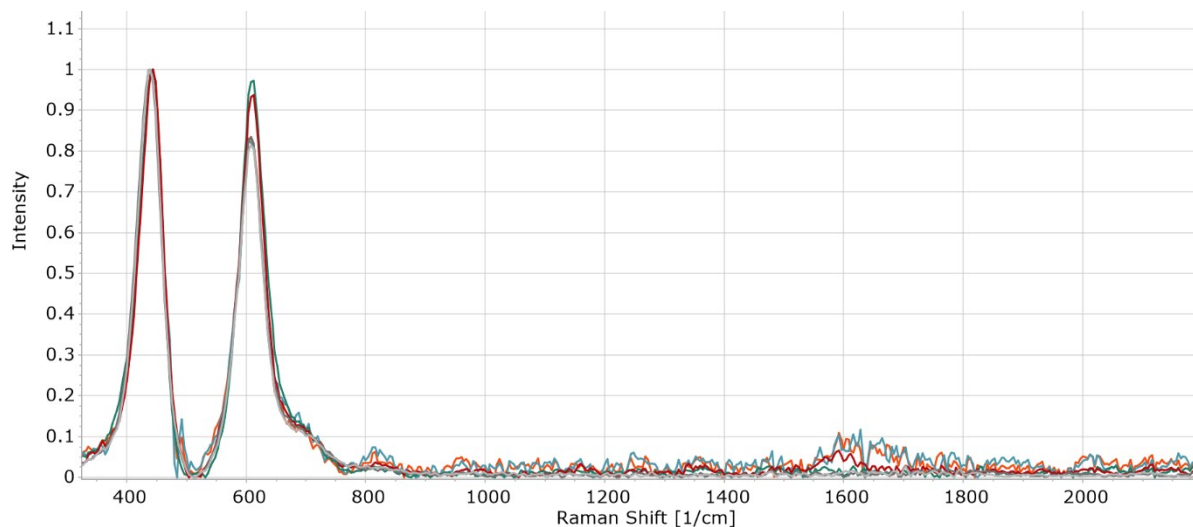


Fig. S2. The stability of the OV_s on the Q-structured TiO_x templates have been assessed over exposure to 360 s at 785 nm Raman wavelength and an intensity of 250 mW/μm² for 120 cycles. As evident no shift and deterioration on the characteristic peaks of the Q-structured TiO_x have been observed. For better observation of the position of the peaks, the acquired spectrums have been normalized.

Bandgap Calculations

The bandgap of the quantum scaled TiO₂ and TiO_x were calculated based on the Kubelka-Munk (K-M or F(R)) method:

$$F(R) = \frac{(1 - R)^2}{2R}$$

where R is the reflectance and F(R) is a function based on extinction coefficient α . the following equation was used to calculate the band gap E_g .

$$\alpha(h\nu) \approx B(h\nu - E_g)^n$$

where E_g is the band gap (eV), h is Planck's constant (J.s), B is absorption constant, ν is light frequency (s⁻¹), α is the extinction coefficient and n is the value for specific transition.

Table S1. Characteristic bands observed in breast cancer and corresponding assignment of biomolecules

Raman bands (cm ⁻¹)	SERS Bands (cm ⁻¹)	Biomolecules	References
622	622	Phenylalanine	1, 2

Raman bands (cm ⁻¹)	SERS Bands (cm ⁻¹)	Biomolecules	References
642 828 853 1620	642 809 839 1620	Tyrosine	2, 3
714	714	Polysaccharides	3, 4
742 1083	742 1083	Phospholipid	3, 5
754 1126 1208	754 1126 1220	Protein	3
875 1447 1556	875 1436–1458 1556	Tryptophan	6
897	897	C-O-C str	3
955	971	CH ₂ rock	3
1002 1028 1103	1002 1035 1103	Phenylalanine	1, 3
1174	1167	Tryptophan, Phenylalanine	6
1230–1282	1230–1282	Amide III	1
1300–1345	1300–1345	Tryptophan, α -helix	3, 6
1404	1404	Glutathione	1
1587	1587	Protein, Tyrosine	3
1603	1603	Tyrosine, Phenylalanine	3, 6
1654	1654	Proteins, Amide I	3

References

1. M. Keshavarz, B. Tan and K. Venkatakrishnan, *ACS Applied Materials & Interfaces*, 2018, DOI: 10.1021/acsami.8b10590.

2. P. Dharmalingam, K. Venkatakrisnan and B. Tan, *Applied Materials Today*, 2019, **16**, 28-41.
3. K. Czamara, K. Majzner, M. Z. Pacia, K. Kochan, A. Kaczor and M. Baranska, *Journal of Raman Spectroscopy*, 2015, **46**, 4-20.
4. J.-K. Yang, I.-J. Hwang, M. G. Cha, H.-I. Kim, D. Yim, D. H. Jeong, Y.-S. Lee and J.-H. Kim, *Small*, 2019, **15**, 1900613.
5. H. H. An, W. B. Han, Y. Kim, H.-S. Kim, Y. Oh and C. S. Yoon, *Journal of Raman Spectroscopy*, 2014, **45**, 292-298.
6. J. Zhang, Q. Huang, G. Yao, Z. Ke, H. Zhang and Y. Lu, *Journal of Molecular Structure*, 2014, **1072**, 195-202.