– Supplemental Information –

Laser Wavelength Selection in Raman Spectroscopy

Mike Hardy[1,] and Hin On Martin Chu[2,3]*

1. *Smart Nano NI, Centre for Quantum Materials and Technologies, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, United Kingdom.*
2. *Advanced Nano-Materials Structures and Applications Laboratories, School of Chemical Engineering, University of Birmingham, Birmingham B15 2TT, United Kingdom.*
3. *Healthcare Technologies Institute, Institute of Translational Medicine, Mindelsohn Way, Birmingham B15 2TH, United Kingdom.*

*mhardy04@qub.ac.uk / smartnanoni.com

Portable Raman systems have a wide-range of spectral resolutions from a low as 1cm^{-1} as high as 14cm^{-1} (Figure S1). Device names are not given in Figure S1 but all specs are readily available online. Information was collected in 2023. Further devices have been surveyed in 2024 but not plotted (details below). All device laser wavelengths are at 785nm, bar device #1. Device #1 is a spatially offset Raman spectroscopy (SORS) device at 830nm.

Often an optimum resolution is provided (Devices #1, #2, #4, #5) while others (Devices #3, #6) give high and low values. The supplier of Device #7 provided an average value. Since the writing of this manuscript, further devices have been surveyed (2024), with given resolutions of 2.5cm^{-1}, <3cm^{-1},and <4/4.5cm^{-1}, respectively (Devices #8, #9, #10, not graphed in Figure S1).

Raman spectroscopy is unusual in the sense that the peaks are given relative to the laser wavelength, and, as explained in the main text, this can obscure thought about the de-excitation wavelength. For example, see Figure S2. Here, three common laser wavelengths are considered, 532nm, 633nm, 780nm alongside the typically analysed i.e. most prominent, Raman peaks associated with popular Raman dye, Crystal Violet (aka gentian violet, methyl violet 10B, hexamethyl pararosaniline chloride; IUPAC name = 4-{Bis[4-(dimethylamino)phenyl]methylidene}-N,N-dimethylcyclohexa-2,5-dien-1-iminium chloride). The de-excitation (or 'scattered') wavelengths in nanometres are provided in the third column of Figure S2 [1].

Figure S3 shows three AI-generated meta-maps pertaining to laser choice in Raman spectroscopy, namely, (a) the progress in laser technology, (b) key themes in this review article (main text), and (c) an AI guide to making the optimum laser wavelength choice.

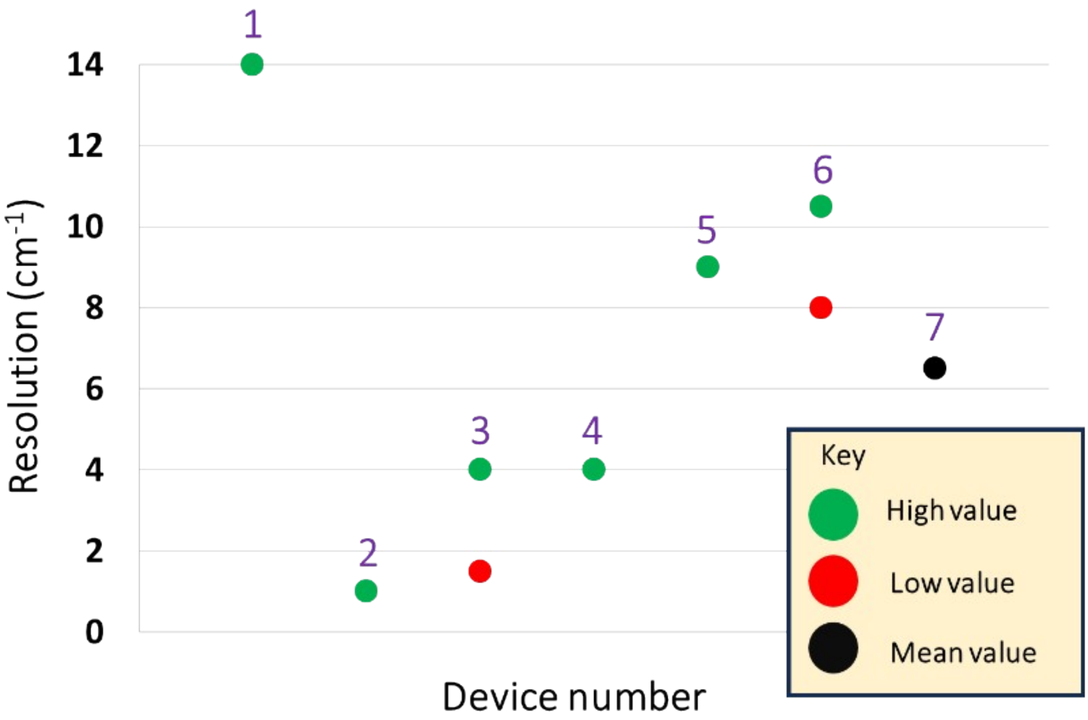

Figure S1. Given spectral resolutions of seven portable Raman devices in 2023.

Excitation Wavelength (nm)	Raman Band (cm^{-1})	Scattered Wavelength (nm)
532	443	545
532	803	556
532	915	559
532	1185	568
532	1617	582
633	443	651
633	803	667
633	915	672
633	1185	684
633	1617	705
780	443	808
780	803	832
780	915	840
780	1185	859
780	1617	893

Figure S2. Common Raman laser wavelengths (532nm, 633nm, 780nm) with significant Crystal Violet Raman bands and corresponding de-excitation wavelengths in nanometres [1]. Reprinted from Hardy, M. © Mike Hardy / Queen's University Belfast 2019.

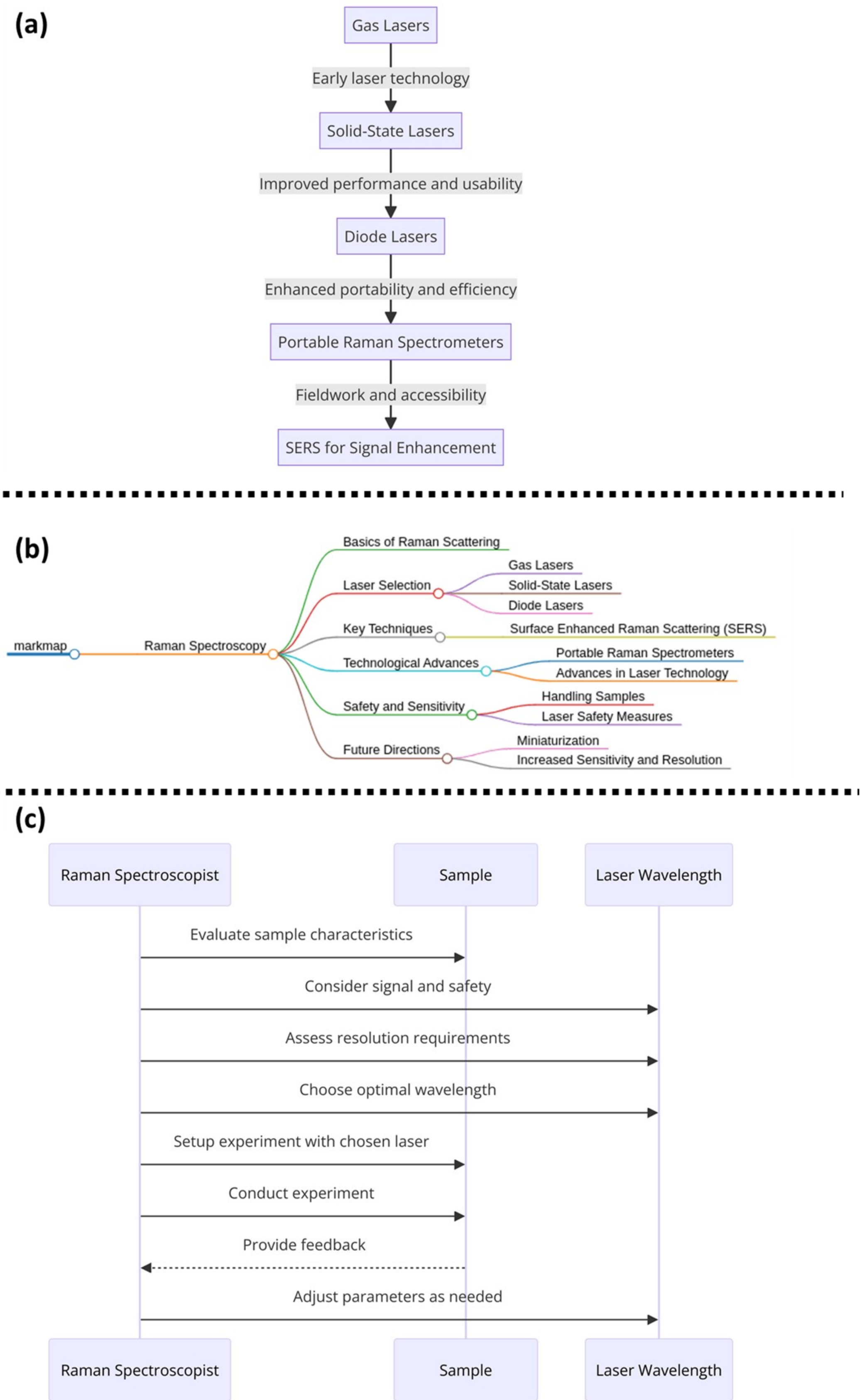
(a)
Gas Lasers
Early laser technology
Solid-State Lasers
Improved performance and usability
Diode Lasers
Enhanced portability and efficiency
Portable Raman Spectrometers
Fieldwork and accessibility
SERS for Signal Enhancement
(b)
markmap
Raman Spectroscopy
Basics of Raman Scattering
Laser Selection
Gas Lasers
Solid-State Lasers
Diode Lasers
Key Techniques
Surface Enhanced Raman Scattering (SERS)
Technological Advances
Portable Raman Spectrometers
Advances in Laser Technology
Safety and Sensitivity
Handling Samples
Laser Safety Measures
Future Directions
Miniaturization
Increased Sensitivity and Resolution
(c)
Raman Spectroscopist
Sample
Laser Wavelength
Evaluate sample characteristics
Consider signal and safety
Assess resolution requirements
Choose optimal wavelength
Setup experiment with chosen laser
Conduct experiment
Provide feedback
Adjust parameters as needed
Raman Spectroscopist
Sample
Laser Wavelength

Figure S3. AI-generated meta-maps pertaining to laser choice in Raman spectroscopy.

(a) Flow chart for progress in laser technology in context of Raman spectroscopy. (b) Mindmap (tree) diagram summarising key areas within this review. (c) Sequence diagram outlining procedure for laser choice in Raman spectroscopy experiments. Diagrams produced by *Diagrams: Show Me* app in Chat GPT 3.5.

Acknowledgements

Thank you to various companies for their time while we were undertaking procurement activities in the Smart Nano lab at Queen's University Belfast, School of Maths and Physics. I am especially thankful to Agilent Technologies for a visit and demonstration.

Thank you to Dr Matthew D. Doherty, School of Maths and Physics, Queen's University Belfast, who originally calculated the scattered wavelength in Figure S2.

References

[1] Hardy, M (2019) *From Fano to Nano: Mechanisms and applications of surface enhanced Raman spectroscopy.* Thesis, Queen's University Belfast.

Photo details (Figure 4, main text)

Ancient Fresco of Religious Figure in Cappadocia – photo by BREAKS OUT.

Photo by Lidija Ostojić: https://www.pexels.com/photo/particles-seen-under-a-microscope-16328960/ cells biological samples

Photo by Fayette Reynolds M.S.: https://www.pexels.com/photo/cell-seen-under-microscope-11198505/ fluorescent samples

Graphene – ChemSketch

Photo by Fayette Reynolds M.S.: https://www.pexels.com/photo/cell-under-microscope-11198491/ - biological samples if fluorescence is desired

Photo by Jeremy Waterhouse: https://www.pexels.com/photo/green-and-black-circuit-board-3665442/ - silicon & inorganic materials

Adam Rędzikowski – zinc oxide photo

Photo by Pixabay: https://www.pexels.com/photo/women-s-black-mascara-63320/ - eye safe