Research Topics Summarization

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Recap

Last time

Okay, well, what have we done last time? Oh yes, *medical applications*...

We unfortunately have decided to **remove** such direction of research topic. Why?

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- Because it is fairly narrow, not a lot of specialized optical physics knowledge can be applied into experiments of such type, at least from a glance.
- Difficulties in gathering resources: Indeed, there seems to be little or too specialized resources (dataset, properties, features, etc.)

So, to mitigate this, we shift our focus to other fields, especially the one that is *closest* to our understanding. This includes, and of course there is, material sciences, solid-state physics, and more.

Considering the improved feasibility of this approach, this presentation will focus on the details about other physics-related experimental field that can apply Raman spectroscopy on, and their potential application that we can get.

Setting up criteria

Criteria categories

Because it is multidiscipline, we have to make up the dimensional criteria analysis (a fancier name for *pick anything, but make it works fairly well for all things considered*) which satisfies the requirement of utilizing the physical technique (Raman scattering), the acting model (machine learning), and applying it to the topic of interest (still the old horse).

So, what constitute the choices? Based on at least current knowledge, we can summarize them as followed.

Raman spectroscopic method (generally, optical physics)

Raman spectroscopy is fairly limited, in what can it affect. However, it is not limited in how can it be utilized. Certainly, for Raman scattering and spectroscopy, we need to know:

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- How many factors can be taken into account which might lead to sample degradation, sample contamination, etc. that ultimately affects how the experiment goes?
- How **costly** it is? What is the cost for operating them?

Machine learning and artificial intelligence

For machine learning, we have two approaches. Or rather, in the sense of *mathematical modelling*. Either **phenomenological** or **mechanistic** modelling can be performed. By doing so, we set ourselves a fair bit of requirements, for minimum:

- (Optional) A comprehensive study or availability to gain partial knowledge of the internal mechanics of the system in analysis (optical physics-specific knowledge might apply)
- Phenomenologically, settings and consideration of **large dataset**, **data availability**, **data interpretability**, and overall *how easy it is to analyse the data, gather the data*?
- Computational complexity: just how much will a certain task costs, and how can it be performed, either pre-training, or after-training? This will inevitably cost you application, for example, high computational complexity for edge device is undesirable.
- Architecture: What type of architecture, either phenomenological or mechanistic modelling will you use?
- What is the **intended goal**? Is the goal or final objective valid of applying machine learning? Are there any specific classical method that works well without using machine learning or artificial intelligence-aid method?
- Cost: How much will it cost, in operating, training, setting up? (Again, too many costs are in consideration?)

Certain topics (for now, it is material science)

Now, for certain topic, they have to satisfy all those above. Then comes down here for a bit of criteria.

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- How much data and support that one specific topic has for both Raman spectroscopy and ML/AI?
- What has been done, what is the main angle of utilization the above topic used in the field?
- Does optical physics have places, or applications that can utilize specialized knowledge of optical physics in said field?

To full realize those criteria, we then have to analyse them, bit by bit.

Observation

So, we want criteria, and we want a topic. There's nothing more than just dive into it, I suppose.

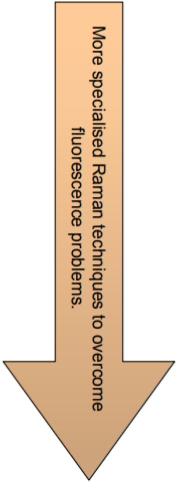
Raman spectroscopy

One of its main potential, from the early day when someone of the same name used solar ray to facilitate the effect is the *fingerprinting property* of Raman spectroscopic method. That is, any given matter will have its own **distinct** Raman spectrum. This leads to the application of **material identification**, **filtering**, *impurities classification (analysis)*, and else that make use specifically the property. Well, a lot of them. But there are also more than just that. Well, let's see for the most normal one.

Types

While Raman scattering, in principle, is just the same, to obtain Raman-like spectrum, we developed a lot of methods.

Those methods will dictates how and what type of data we gain, and also the form of the system, especially the parameters of the given spectroscopic system if we are trying to do ML application - they need all the parameters.



Raman Technique	Typical Laser Wavelengths
Dispersive/ Visible	Visible Lasers: 488, 514, 633 nm
Dispersive/ Near Infra-Red (NIR)	NIR Lasers: 785, 830 nm
SERS	Any visible or NIR Lasers
FT-Raman	Nd: YAG Laser: 1064 nm
UVRR	UV Lasers: 230, 206.5 nm

Figure 2.1. *Technological Advances in Raman spectroscopy*

Figure 1: Technological Advances in Raman spectroscopy. This is taken from, NPL Report DQL-AS 012, which has protein as the other axis, which is omitted.

Spontaneous Raman spectroscopy

The usual, traditional Raman spectroscopic method.

Advantage Spectral details, classification.

Challenges Slow as heck.

Sample preparation No.

Full spectrum Yes.

Resonance Raman Scattering (RRS)

Unlike other enhancement effects, resonance Raman only amplifies Raman scattering from a specific vibrational mode of the molecule in resonance with the excitation illumination. Other modes and molecules in the sample are not affected.

- **Advantage** More signal, specific targets.
- **Challenges** Only possible with some molecules (like, coloured molecules?)

Sample preparation No.

Full spectrum Yes, some band is enhanced.

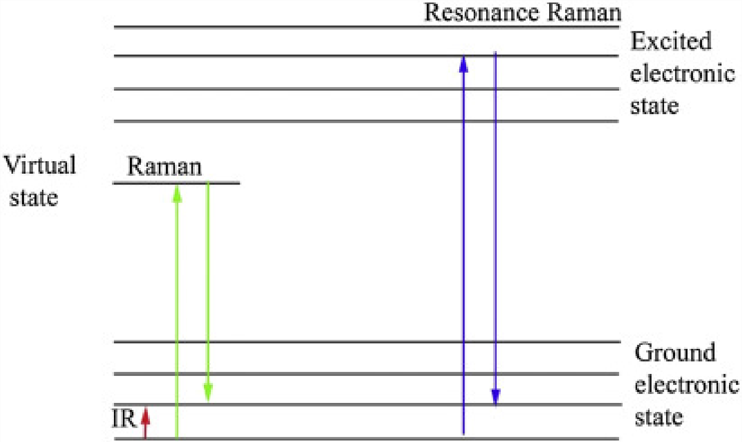


Figure 2: Illustrative difference of RRS method.

Coherent anti-Stokes Raman scattering (CARS)

The development of coherent Raman microscopies came as a solution to the slow imaging inherent to spontaneous Raman scattering-based techniques.

- **Advantage** Very fast imaging.
- **Challenges** Costly, signal depends on concentration of $O(n^2)$ scale.

Sample preparation No.

Full spectrum Possible with more complex instrumentation.

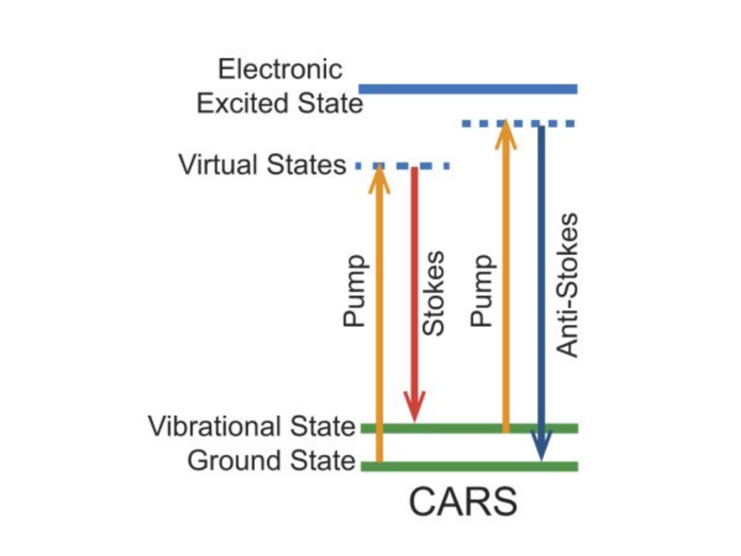


Figure 3: Illustrative difference of CARS method.

Stimulated Raman scattering (SRS)

Stimulated Raman scattering (SRS) describes a family of techniques first discovered and developed in the 1960s.

While spontaneous Raman scattering is an incoherent technique, SRS is a coherent process, and this fact provides several advantages over conventional Raman techniques, among which are much stronger signals and the ability to time-resolve the vibrational motions.

Advantage Very fast imaging, signal depends linearly on concentration

Challenges Costly.

Sample preparation No.

Full spectrum Yes, but complex selection rules cause non-standard spectra.

Some others...

Alright, it is too long now. So we will list the perhaps others approach, both again, with their drawbacks and advantages.

- Surface enhanced Raman scattering (SERS).
- Tip-enhanced Raman scattering (TERS).
- Spatially offset Raman spectroscopy (SORS).
- Transmission Raman spectroscopy.
- Selective scanning Raman spectroscopy (SSRS).

But, we left out, well, Fourier Transform Raman Spectroscopy (FT-Raman or FTRS)

Fourier Transform Raman Spectroscopy (FT-Raman)

Fourier transform (FT) Raman spectroscopy involves the use of a multiplexing spectrometer, such as a Michelson interferometer, to detect and analyse the scattered radiation from a sample. Usually, it operates on the near-infrared range ($\sim 1064\ nm$), and use interferometer plus Fourier transform to convert the interference pattern to the original spectrum. This gives it:

- Super low fluorescence effect.

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- Super low fluorescence effect.
- Very high accuracy of the x-axis (shifted wavenumber).
- Well-suited for bulk sample analysis.

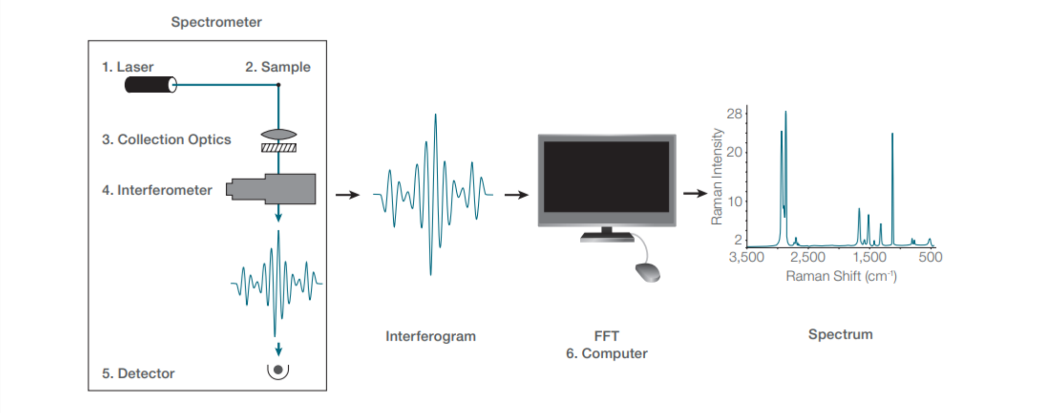

Figure 4: Illustrative operating chain of a FT-Raman spectroscopic setting.

Indeed, the above makes FT-Raman a very viable and perhaps most practical experimental setting we can have, in the modern range. It has plenty advantages, and disadvantages, however, to dispersive Raman spectroscopy (DRS), but the two can complement each other:

- FT-Raman is the best choice in situations where samples fluoresce or are likely to contain minor impurities that may fluoresce.

Indeed, the above makes FT-Raman a very viable and perhaps most practical experimental setting we can have, in the modern range. It has plenty advantages, and disadvantages, however, to dispersive Raman spectroscopy (DRS), but the two can complement each other:

- FT-Raman is the best choice in situations where samples fluoresce or are likely to contain minor impurities that may fluoresce.
- Dispersive Raman spectroscopy has been applied to many types of samples, especially like single crystals study. Its main advantage is micron-level spatial resolution, higher sensitivity obtained at visible laser wavelengths.

Applications of Raman Spectroscopy

The non-ML application

Raman spectroscopy is mentioned to be particularly effective, if not widely used in material sciences with their successes. We first review some of the general applications first, in which there are plenty.

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The non-ML application

Generally, Raman spectroscopy is applied in:

- Inorganic and minerals — Identification, analysis, quality check and control.
- Art and archeology — Non-destructive sample analysis.
- Polymers and emulsions — identification, structure composition, curing, and in studying polymer composites.
- Colour — Analysis of coloured molecules.
- Electronics: Used for analysing electrophotography dyes, and studying such materials in devices.

Still the non-ML application

Those are some typical normal application for Raman spectroscopy. Now, that is all good, but what about specifically material science? We found specifically some of the same interest. But what is the specific application for material sciences and its relating in a sense field: Well, we identified several interesting applications for a lot of them.

Material analysis

This includes a variety of materials and application:

- Ge quantum wires, inorganic or organic materials.

In the context of **earth and material science** in conjunction, such materials in analysis expanded to crystalline spectra, for example, of amorphous SiO2.

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- Ge quantum wires, inorganic or organic materials.
- Material identification of basic characterization, for example, in **amorphous materials** (glass, for example), or characterization of GaN quantum dots.
- Layers material (Ni et al. (2008), Sorkin (2014)) in, for example, bulk graphite (HOPG).

In the context of **earth and material science** in conjunction, such materials in analysis expanded to crystalline spectra, for example, of amorphous SiO2.

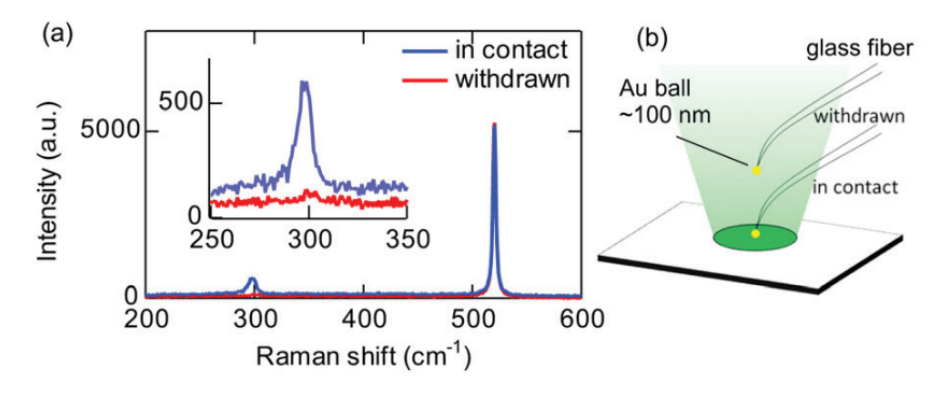

Figure 5: (a) Raman spectra of a single Ge nanowire on a SiO2/Si substrate with the AFM tip in contact (blue line) and with the tip withdrawn (redline). (b) Experimental setup.

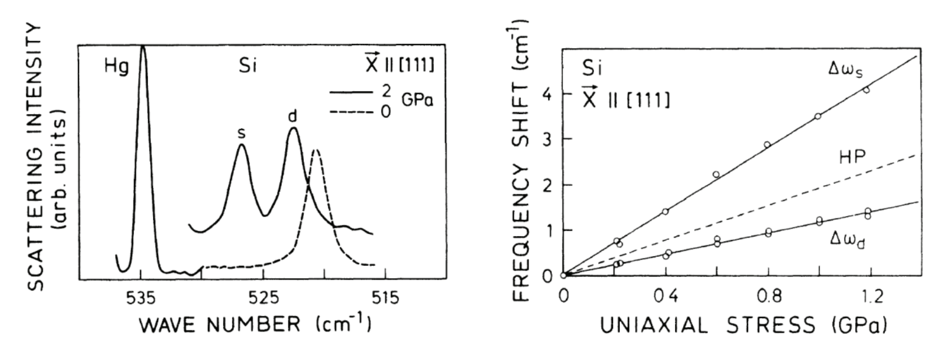

Figure 6: Left panel: Singlet and doublet Raman peaks of silicon when an uniaxial stress is applied along the [111] direction. Right panel: Phonon shift of Si with uniaxial stress.

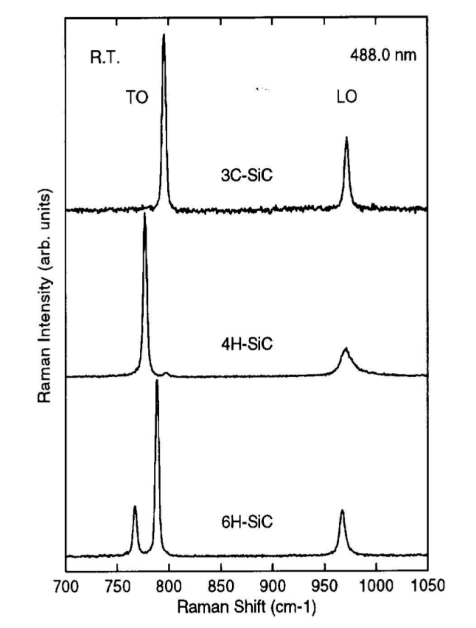

Figure 7: Distinction of different silicon carbide polytypes using Raman scattering.

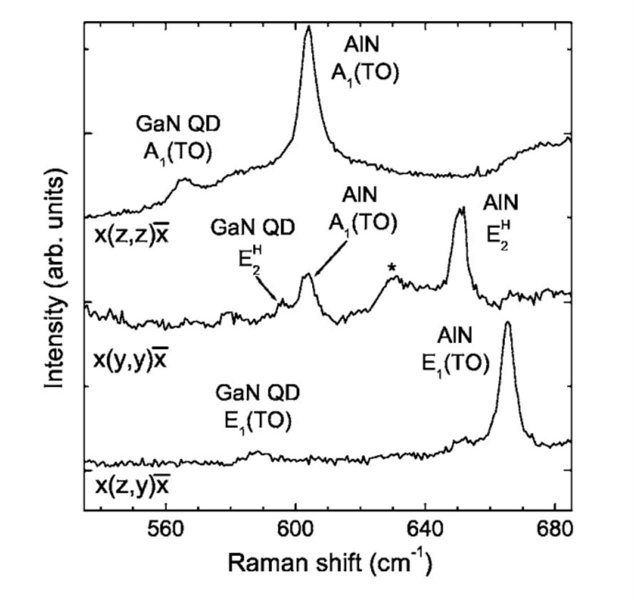

Figure 8: Different phonon modes of GaN quantum dots embedded in AlN.

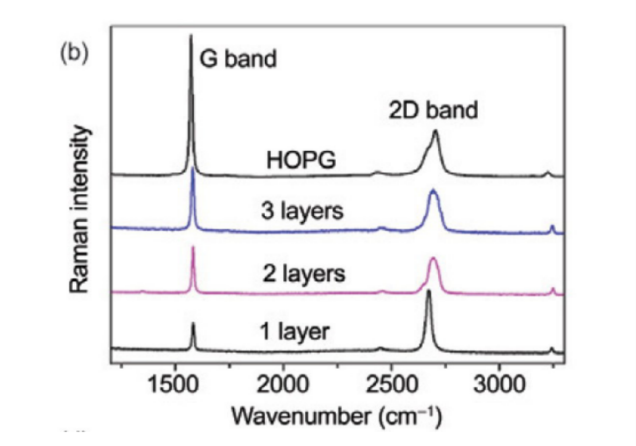

Figure 9: Raman spectra of 1, 2, 3 graphene layers compared with that of bulk graphite (HOPG)

Optical effects

Materials can have various effects observable by Raman spectroscopy.

- Isotopic effect can be extracted meaningfully using Raman frequency [Windulle et al. (1999)] for Ge decomposition.

[1] An effect observable, called the surface optical phonons, where the bulk materials surface produces visible new phonon modes related to the surface, which plays a large role for few layers of materials, or quantum wires of low-dimension.

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- Isotopic effect can be extracted meaningfully using Raman frequency [Windulle et al. (1999)] for Ge decomposition.
- Raman can be used to extract meaningful information [Cantarero (2013), Moller et al. (2011)] about the TO, and LO phonon in case of the effect called **surface optical phonons**[1]

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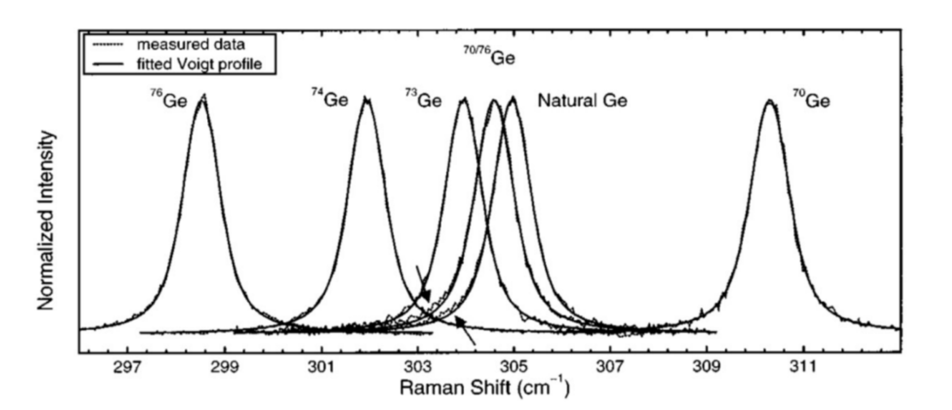

Figure 10: Raman shift of natural Ge and enriched Ge isotopes. From the figure we can check that the shift if basically proportional to the square root of the isotopic mass.

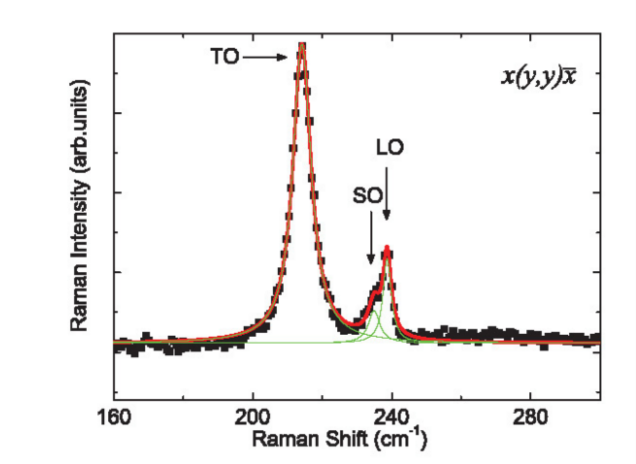

Figure 11: Raman shift of an isolated InAs nanowire and the corresponding fit.

Electronic density

Electronic density of states can also be analyzed, for doped semiconductor, which gives the electron concentration of a semiconducting material, for example, in a book chapter of Klein (1998) on GaAs.

Silicon can be doped much more than such, and hence, another way for Raman spectra here to be observed, or extracted, is during the process of **energy concentration increment**: because then, at some point the electronic background will interfere with the phonon, and the shape of the phonon deviates from typical profile, giving the **Fano line-shape** for all kind of excitation spectra.

This is more thoroughly studied in [Belitsky et al. (1997)] treatment on the theory of Raman scattering due to interaction of phonons with electronic background.

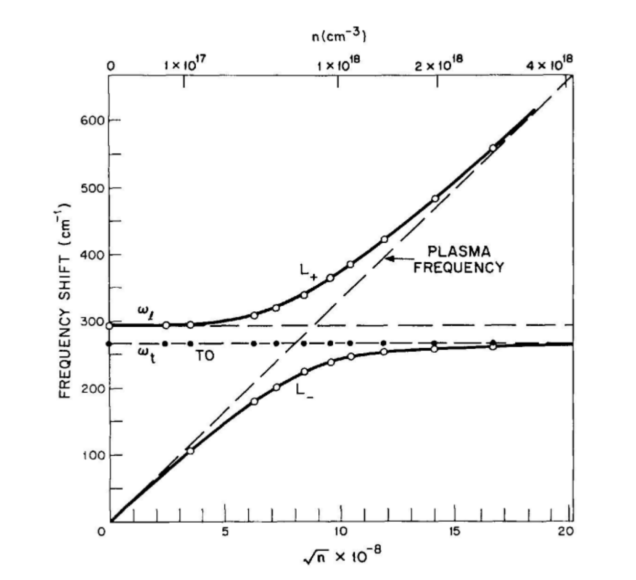

Figure 12: Frequency shift of the GaAs phonons in a heavily doped sample due to the coupling of the LO phonon with the plasmon.

More – layering materials

A particular application can be found about Raman spectroscopy on layered structure. For example, [18] gives a particular interesting approach to Raman Spectra of Monolayer, Few-layer, and Bulk $\mathrm{ReSe_2}$ semiconductor.

Using such, they can determine layer thickness, crystal position and orientation, monolayer regions. With supporting theory, they can even calculate **electronic band structure** and Brillouin zone layer, and scattering intensity.

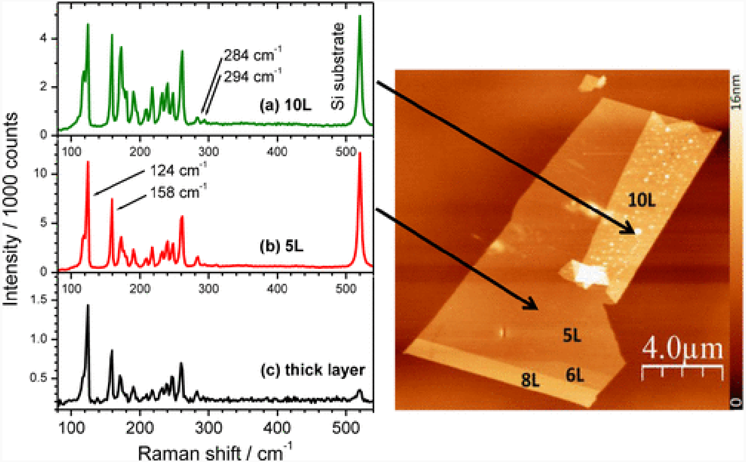

Figure 13: Raman scattering spectra of ReSe2 on a SiO2/Si substrate for (a) 10 layers; (b) 5 layers, and (c) a thick flake.

Applying machine learning

Machine learning on spectroscopy

Machine learning, specifically, the phenomenological approach that has been there since eternity (well, 1920s).

On its own, the word phenomenological speaks it all - it use data, or rather, observations without knowing the internal mechanics (the black-box interpretation approach) to form model that mimic said behaviour observed given in the dataset.

Machine learning on spectroscopy

Often, the dataset $\mathcal{S}$ will typically be formed of criteria or assumptions, probability distribution, and other statistical descriptions. Generally speaking, they learn from data.

When working with machine learning models, usually, there are two types of widely used methods. First, is the *classical machine learning models*, or rather, models unrelated to the general scheme of neural network. And second, is the *deep learning model*, which obviously, formalize the neural network architecture to everything conceivable in the network.

Machine learning on spectroscopy

Well, see for yourselves why they would like to use more deep learning than classical — it is also proven, in certain cases, that deep learning model works better than classical setting.

We only have a few concerns in such sense of operating and working with machine learning models. But really, aside from the criteria... not so much can be said about it.

Machine learning on spectroscopy

Ultimately though, this section overlaps with what I was about to present in the well, past essay, so we will skip over that one. Or, we will somewhat ‘borrow’ it from that essay of mine (eh, I hold the copyright anyway).

Based on use cases of Raman spectroscopy, application of machine learning and deep learning [14, 3] is divided into four main categories:

1. Preprocessing data.

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1. Preprocessing data.
2. Spectral **classification**
3. Spectral regression.
4. Spectral region **highlighting**

Classical learning model

Details depends on their usage, but most traditional works with the same structure. Most of them, however, utilizes variable primitive analysis types and architectures. Classically, they are:

- Principal component analysis (PCA), SNR denoising, etc. (preprocessing) + partial least square (PLS) model - *regression analysis*
- PCA + SVD for Breast Cancer diagnosis (Manoharan et al.) [3, 11]
- Support vector machine for NIR-Raman (Widjaja et al.) [3]

Modern deep learning

For more recent application of deep learning, a comprehensive list of both usually appearing models are presented. Bottom entries are some of those. [15]

Bayesian	A classification technique based on the Bayes theorem, where the prior probability distribution is selected and then updated to obtain the posterior distribution.
Artificial Neural Network (ANN)	A mathematical model that simulates the brain's neuronal activity as a set of connected input/output units, where each connection has a weight associated with it.
Convolutional Neural Network (CNN)	A class of feedforward neural networks with convolutional computation and deep structures. It is usually applied to analyze visual imagery.
Recurrent Neural Network (RNN)	A class of neural networks with short-term memory, suitable for processing a range of time-series related problems such as text.
Probabilistic Neural Network (PNN)	A neural network technique based on the Bayesian decision rule that is widely used in classification problems.
Generative Adversarial Network (GAN)	A novel adversarial generative model architecture that learns to generate new data with the same statistics as the training set.

Figure 14: A list of recent modern *deep learning* architecture in applications.

Modern deep learning

We focus on the following:

1. Convolutional Neural Network (CNN - and most popular).
2. Bayesian Statistical Model (Most complex, very accurate.)
3. Physics-informed neural network (PINNs - state-of-the-art for physics application).

Convolutional networks (CNN)

Convolutional neural network is the most popular model architecture in papers and projects on Raman spectroscopic analysis ($\approx 57.25\%$) [16, 3, 4, 8].

Most of them are concerned with 1D case, however, from our previous assumption.

Mathematically, a typical 1D CNN operation can be simplified as:

$$y(i) = \sigma\left(\sum_h x(i+h)k(h) + b\right) \tag{1}$$

where x is the 1D input, y is the output, k is the learnable kernel, b is the bias term and σ is a nonlinear operation. Within each layer, we also have the pooling layer for down-sampling spectra:

$$Y_{x',k} = \max_{0 \leq m \leq s}(X_{x \cdot s+m,k}) \tag{2}$$

where s is the pooling filter size, x and x' are wavenumber indices of the input and output spectra, respectively.

Lastly, usually, there exists a fully connected layer at the end of the convolutional steps:

$$Y_{k'} = b_{k'} + \sum_{x \times k} Fw_{k', x \times k} X_{x \times k}$$

where Fw denotes the weights of the fully connected layer.

Diagrammatical View

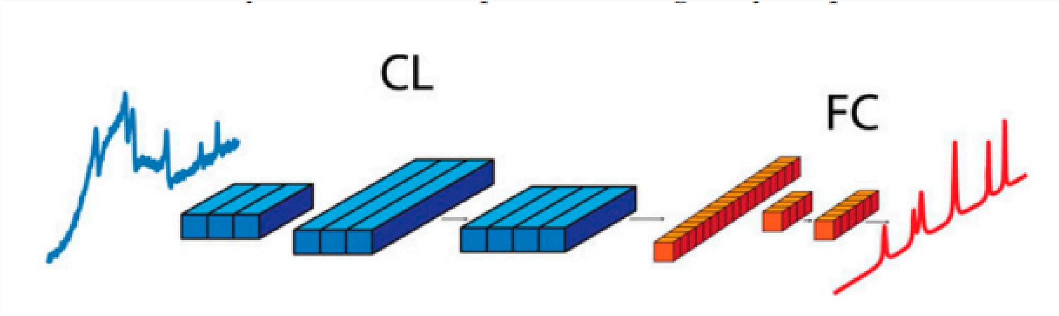


Figure 15: Diagrammatical, simplified view of the underlying structure for the CNN-Raman network. In this case, it is for data preprocessing, such as **baseline correction**. Adopt from **Ruihao** [3]

Usages

CNN is used in all cases of interest mentioned above, from preprocessing to highlighting, which *specifically* utilizes the convolutional logics of the network. Preprocessing also taken large parts of papers regarding CNN application with widespread successes. [3]

Performance

Within various cases, it presents good efficiency, and well-controlled behaviours [3, 4, 5, 15], beats out classical machine learning techniques.

Table 2: Test accuracy of the compared machine learning methods on the baseline corrected dataset

Methods	KNN(k=1)	Gradient Boosting	Random Forest†	SVM(linear)	SVM(rbf)	Correlation	CNN†
Top-1 Accuracy	0.779±0.011	0.617±0.008	0.645±0.007	0.819±0.004	0.746±0.003	0.717±0.006	**0.884±0.005**
Top-3 Accuracy	0.780±0.011	0.763±0.011	0.753±0.010	0.903±0.006	0.864±0.006	0.829±0.005	**0.953±0.002**
Top-5 Accuracy	0.780±0.011	0.812±0.010	0.789±0.009	0.920±0.003	0.890±0.007	0.857±0.005	**0.963±0.002**

Figure 16: Performance evaluation of a typical CNN model on baseline corrected data. Adopt from [10]

Performance

Table 3: Test accuracy of the compared machine learning methods on raw dataset with or without baseline correction methods

Methods	KNN(k=1)	Gradient Boosting	Random Forest†	SVM(linear)	SVM(rbf)	Correlation	CNN†
Raw	0.429±0.011	0.373±0.019	0.394±0.016	0.522±0.011	0.434±0.012	0.310±0.007	**0.933±0.007**
Asym LS	0.817±0.010	0.773±0.009	0.731±0.019	0.821±0.012	0.629±0.016	0.777±0.013	**0.927±0.008**
Modified Poly	0.778±0.007	0.740±0.016	0.650±0.016	0.785±0.014	0.629±0.016	0.734±0.013	**0.920±0.008**
Rolling Ball	0.775±0.009	0.737±0.008	0.689±0.018	0.795±0.011	0.624±0.013	0.730±0.010	**0.918±0.008**
Rubber Band	0.825±0.007	0.792±0.015	0.741±0.009	0.806±0.015	0.620±0.010	0.789±0.010	**0.911±0.008**
IRLS	0.772±0.010	0.710±0.008	0.675±0.007	0.781±0.011	0.614±0.010	0.711±0.011	**0.911±0.008**
Robust LR	0.741±0.009	0.694±0.008	0.667±0.012	0.759±0.013	0.600±0.013	0.696±0.011	**0.909±0.007**

Figure 17: Performance evaluation of a typical CNN model on non-baseline corrected data. Adopt from [10]

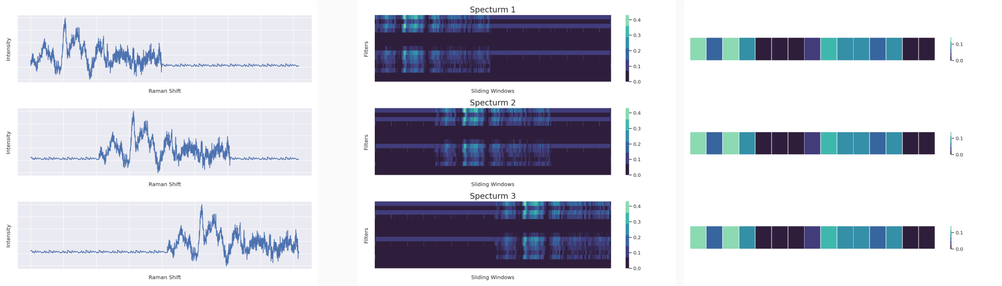
However. . .

From a **visual perception** perspective, Raman spectrum resembles a signal-like waveform. [16, 8]

However, Raman spectra is an energy distribution plot, which might not suitable for normal utilization of CNNs. [8]

Specifically, it discards the time-domain locality of the spectrum, which is crucial for Raman spectra.

However. . .



(a) (b) (c)

Figure 18: Analysis of CNN for a Raman spectrum input. Reproduced from [8]

Solutions (allegedly)

Several solutions has been proposed to resolve this particular problem, and some else more on-site specific, or situational-specific. The most recent, and can be said, potent, is *RamanNet* [8].

Instead of 1, we have the MLP:

$$y(i) = \sigma(W_{f(i)}^T + b) \equiv \sigma\left[\sum_h x(i+h)k_{f(i)}(h) + b\right] \tag{3}$$

Where $W^T x$ is equivalent to the 1D convolutional operation with proper relation between W and the kernel k. The small index $f(i)$ indicates that they are position-dependent. This is implemented with a **sliding window** in the architecture.

Evaluation

Testing this architecture against classical technique (SVM) shows non-trivial performance boost.

Table 2: Results on COVID-19 Dataset

COVID-19 vs Suspected			
Method	Accuracy	Sensitivity	Specificity
SVM	87 ± 5	89 ± 8	86 ± 9
RamanNet	93 ± 3	97 ± 4	90 ± 6
COVID-19 vs Healthy			
Method	Accuracy	Sensitivity	Specificity
SVM	91 ± 4	89 ± 7	93 ± 6
RamanNet	95	95 ± 4	96 ± 3
Suspected vs Healthy			
Method	Accuracy	Sensitivity	Specificity
SVM	69 ± 5	70 ± 9	66 ± 9
RamanNet	82 ± 6	77 ± 15	87 ± 11

Evaluation

Similarly, on Melanoma Dataset compare to CNN.

Table 3: Results on Melanoma Dataset

	$-NH_2$		$-(COOH)_2$		-COOH		All	
Fold	RamanNet	CNN	RamanNet	CNN	RamanNet	CNN	RamanNet	CNN
1	**100**	97.42	**100**	100	**99.35**	94.19	100	100
2	**99.35**	96.13	**99.35**	98.71	**98.71**	96.12	100	98.71
3	**100**	95.45	**100**	98.05	**99.35**	87.01	100	100
4	**100**	97.40	**100**	98.70	**96.75**	96.10	100	99.35

Evaluation

CNN models have *moderate* accuracy, average size-to-performance, adaptable to various scenarios, and in some way, very *natural* when it comes to adapting Raman interpretation.

Adaptability is best expressed by the *RamanNet* itself - with simple modification comes great improvement and mitigation of earlier issues - very easy to use.

Bayesian system

Another way entirely, is to use Bayesian modelling to instead sample and quantify the Raman spectroscopic system instead. [12, 7, 6].

As the name suggested, those models are highly statistical, and often characterized by certain **statistical processes**, often stochastic, or in the case of [7], it can include a sequential Monte Carlo sampler.

Bayesian system

Performance-wise, it is surprisingly effective:

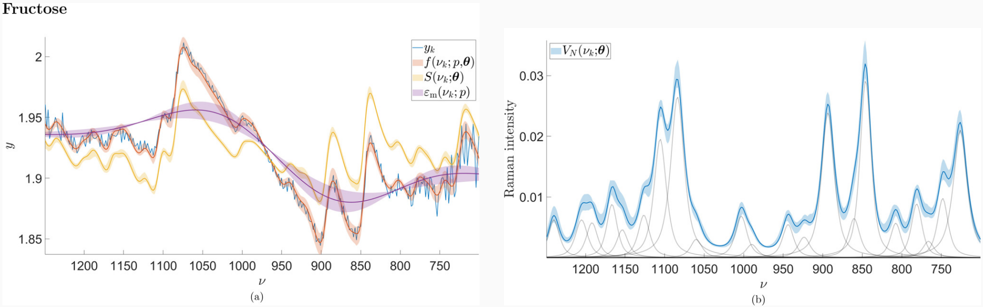


Figure 19: (a) Obtained 95% predictive intervals for y_k, f, S, and ϵ_m shown in blue, red, yellow, and purple respectively for a CARS measurement of a adenosine phosphate sample. (b) Obtained 95% predictive intervals for $V_N(v_K, \theta)$ and means of each individual line shape $V(v_k, \theta_n)$ for the adenosine phosphate sample. Reproduced from *Teemu et al.* [7]

Bayesian system - disadvantage

The disadvantage however, comes at a cost of:

1. High complexity, less flexibility.
2. Large complex dataset required (multipage prior distributions).
3. Out of trend/fashion in comparison to ANN/DNN.

However, if the need for static, complex settings (or mixture) arises, Bayesian can *squeeze* out the most in many situations.

The PINNs

The last model of discussion is the more recent approach of Physics-informed network - PINNs for Raman spectroscopic setting.

This type of Theory-Trained Network (TTNs) are especially useful for any dynamic physics system, and the scattering phenomena is one of such.

The PINNs

This development is natural, however. PINNs are effective in multi-scattering simulation [13] and was particularly useful in computation of quantum-based spectrums [1].

[2] and [9] explored these options quite thoroughly. However, the most prominent, or at least effective model is the **SRS-Net** [17] (Song et al., 2024), originally intended for *nonlinear* fibre-optic systems' Raman scattering.

This system is inherently difficult, and specialized, customized setting is very much required [17]

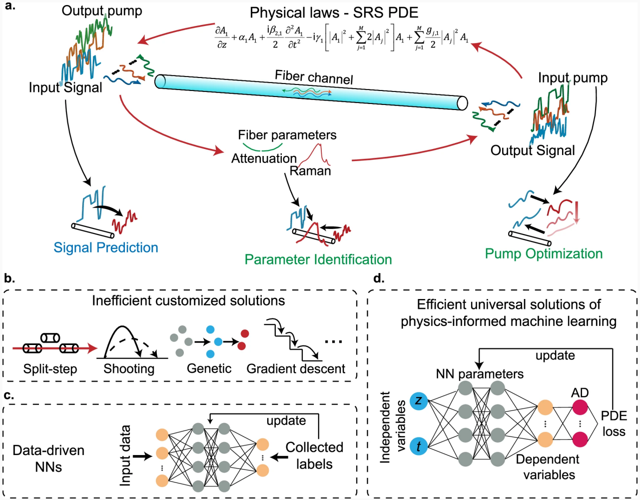


Figure 20: (a) The complex relationships among signals, pumps, and SRS's PDE. (b) Inefficient customized solutions using multiple classical numerical methods. (c) Data-driven NNs trained by collected labels. (d) Efficient universal solutions using physics-informed machine learning and AD.

Performances

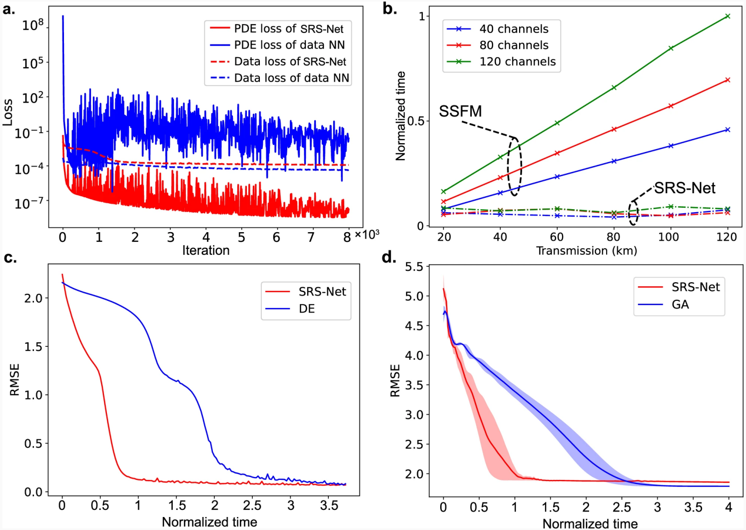


Figure 21: Results of SRS-Net physics consistency, testing speed, and performance comparison to genetic engineering (GA), split-step Fourier method (SSFM), and data NN. Reused from [17]

The feasible idea

The feasible idea

Okay, that is a long analysis. So, what do we have in hand for now?

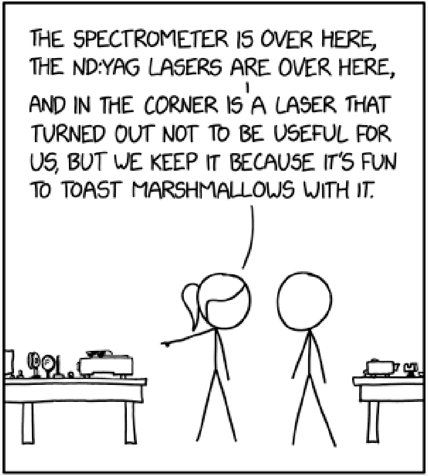
We have some opinions and views on the topic, as accordance to the tradition.

Data availability

It is observed (Ewen, Geoffrey, 2005) that Raman spectroscopy is **inherently expensive**. Tradeoffs will happen with various techniques and spectroscopic setting, however, it is imperative to consider this beforehand. Data availability is indeed a problem, as taking into account the time complexity of acquiring samples, the amount of sample preparation and controlled sample setting, and overall, the cost of said sampling process is not cheap.

Data availability

Well, seriously, I even got that one time when I thought I can even **buy the Raman kit**. Man, that was stupid.



EVERY LAB IN EVERY FIELD HAS SOME PIECE OF EQUIPMENT LIKE THIS.

Data availability

To combat this, it is also observed from researches, that we can use either quantum simulation with potential aids from quantum machine learning model to synthetically create samples, based a small pool of sample as exemplary.

More simply, we can use diffusions models, or any signal-processing model that can capture the relative, statistical intrinsic property of sample and its Raman spectrum, and hence applies noise (like Gaussian $\mathcal{N}(\mu, \sigma)$) to synthetically generate sample of varied spectrum (retaining the characteristic, however).

Topic consideration

After some thoughts, we think for ourselves — it ought to be good to consider our topic choosing procedure in a bit **level-like** fashion.

By this, though, I would like to think about it in a more dimension like fashion. What if we are to increase gradually the dimension of the Raman spectrum?

1D – typical Raman analysis

There are already a lot to do for Raman of 1-dimensional – or point spectral scan. A lot of normal application is also about 1-dimensional spectrum. Remember [8]? RamanNet is utilized mostly for, well, 1-dimensional spectrum.

For its application, we have not that much to improve. Generally, we can choose our topic of consideration to be in those fields of possible application.

1D – typical Raman analysis

For our specific problem on material science, semiconductor (maybe?), solid state physics, there would be possible the perhaps hybrid option of point-to-point analysis. Or rather, by using pinpointing 1-dimensional Raman spectroscopy, what can we tell about the structure of the system, and how can we utilize such data for machine learning algorithm to identify, extract and evaluate such data?

This is perhaps interpreted as similar to **geological probing** – where instead of scanning the entire field or mountain range, they analyze **specific points** on the landscape. Can we do such?

It also helps that it offers the usage of **Raman microscopy**, which is either 1D probing, or very small section ($50 - 100\ \mu m$ deep).

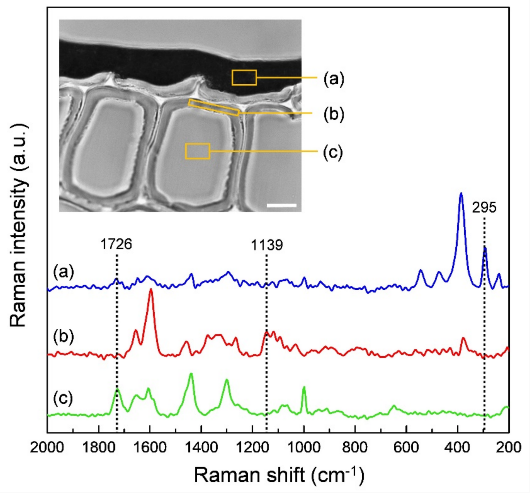


Figure 22: Application of Confocal Raman Microscopy on Wood cross-section.

Layering

An aspect that can be said about Raman spectroscopy of such point, is the fact, or rather, the interesting issue that will persist in ideas and research problem in the future is the issue of **layers** - or rather, sub-surface Raman analysis. Can Raman do it? Yes, perhaps rather interestingly so.

> *any solid chemicals are delivered in white plastic containers, often made of titanium dioxide-filled polyethylene. The filler material scatters light and makes the plastic appear opaque. Laser light cannot be focused inside such containers due to the strong scattering, precluding the use of conventional Raman backscatter measurement designs. Using STRaman, both the 785-nm excitation laser and the Raman scattered light can penetrate the plastic wall through a diffuse scattering mechanism, and its large effective sampling depth allows such materials to be interrogated and identified.*
>
> *(M — Jun Zhao, Katherine A. Bakeev AND Jack Zhou, B&W TEK LLC.)*

The full paper can be found here

And, it's not that bad!

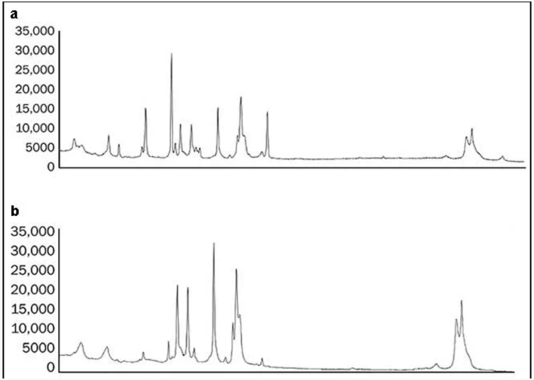


Figure 23: See-through Raman spectroscopy (STRaman) identification of sodium benzoate through a white polyethylene bottle; spectrum measured through the bottle using the STRaman technology (a); spectrum measured with a standard Raman configuration (b)

Layering

Extending this notion (find papers and resources on it to utilize at least) will be interesting. This is also particularly true for 1-D data - it balances out the ergonomic.

This also offers us to be able to extract layering information from 1D method of particular material or structure.

1D – typical Raman analysis

Coming back, for 1D system, of the ergonomic, probing is somehow, perhaps one of the best (cost-wise) approach to the problem. This is because it can give us the separation of the issue into 3 sections:

- Normal microscopic imaging region processing.
- Raman probing processing.
- Physical interpretation and optical interpretation.

If able, real-time system can be very helpful in simulation of complex changing material.

1D – typical Raman analysis

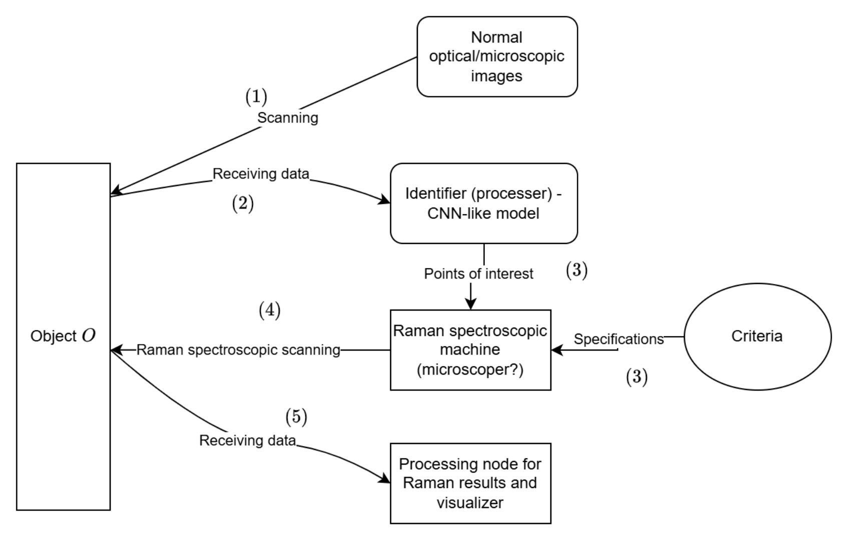


Figure 24: A simple conceptual flowchart (somewhat) about their operations.

Hyperspectral – 2D

It is a valid consideration that hyperspectral imaging for a far-reaching sample might prove useful, since even though we have been heuristically, and blindly (somewhat) using CNN and its derived class. By then, the data captured using Raman spectrometer is not utilized, or rather, too few to be utilized by the architecture itself.

Granted, they are of the wavelet, signal-like system, but typical analysis in such aspect only leaves data in 1D, which is undesirable, and perhaps there are better alternatives than just plain CNN for various tasks. Though, data availability, data acquisition ability, and the cost of operation will eventually be a bigger concern.

Hyperspectral – 2D

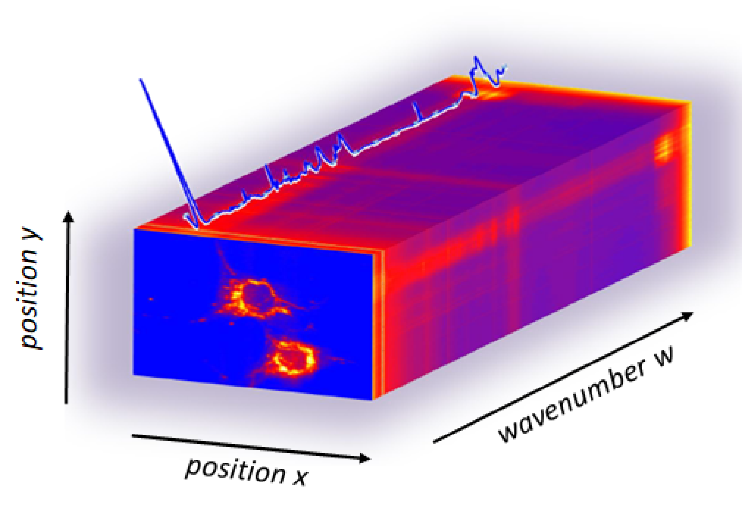


Figure 25: A simple conceptual flowchart (somewhat) about their operations.

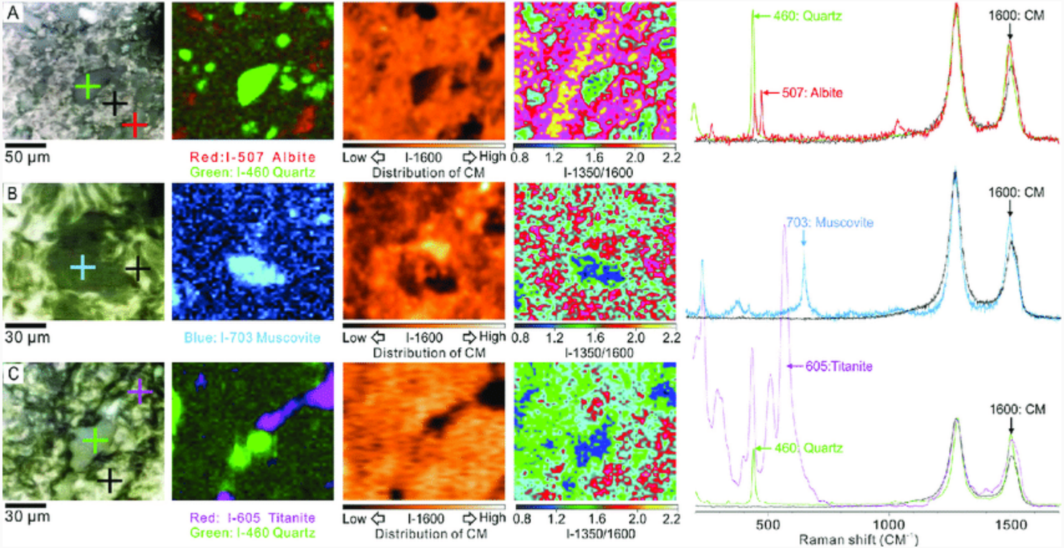


Figure 26: Selected Raman spectra and Raman hyperspectral maps of Contact-CM and Matrix-CM in relation to various mineral phases within the massive organic-rich parts of the Zaonega Formation. [Yuangao Qu et al., 2020]

3D – Raman 'super'imaging

A lot of the ideas we mentioned, target the specific new technique of Raman (maybe), the **3D Raman imaging**.

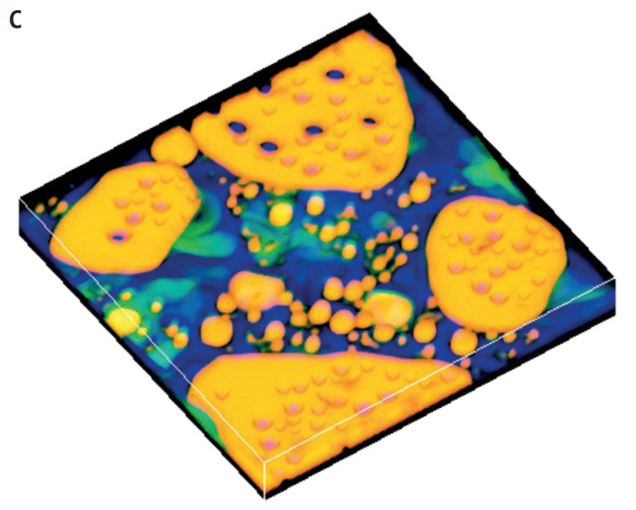
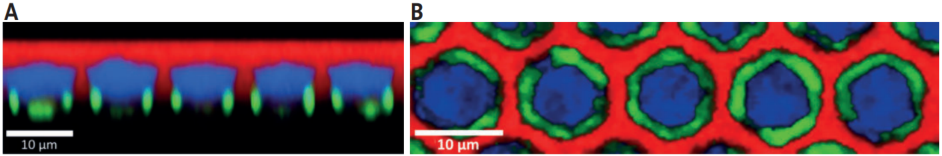


Figure 27: 3D confocal Raman image of the emulsion of the identified components: alkane (green),



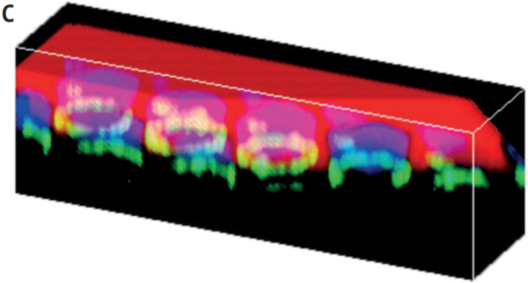
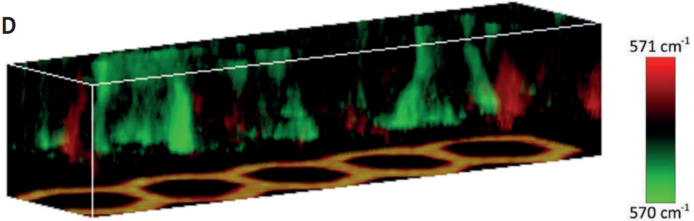


Figure 4: 3D Raman imaging of a GaN crystal. *Sample courtesy of Dr. Eberhard Richter (Materials Technology Department of the Ferdinand Braun Institute, Berlin, Germany).* ***A:*** *Depth scan (x-z plane) along a line of substrate pits. Scan range: 60 x 20 µm^2; 240 x 80 pixels.* ***B:*** *Example 2D Raman image (x-y plane) extracted from the recorded image stack (C).* ***C:*** *3D Raman image of the sample volume. Scan range: 60 x 15 x 20 µm^3; 180 x 45 x 20 pixels. At the front right corner, a part of the structure has been removed for better visibility.* ***D:*** *Strain fields in the crystal, revealed by shifts of the E_2^{high} Raman peak. The image in the bottom plane indicates the positions of the substrate's pits.*



Thank you

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