LIBPhys | Projecto de Tese de Doutoramento | Engenharia Biomédica

Development of an assessment tool for dental diagnostics using Raman spectroscopy

Objectives:

Raman spectroscopy has proven to be a valuable tool for the evaluation of the soundness of dental tissues. However, the accuracy of diagnostics is dependent of the reliability of the spectra evaluation and of the significance of the data acquired in the measurements. In this thesis we propose the implementation of a novel spectra evaluation approach, using Machine Learning algorithms based on Deep Learning´s Convolutional Neural Networks. This tool will then be implemented in Raman device that is currently being developed at LIBPhys: a dedicated Raman probe designed and adapted to a Raman benchtop spectrometer, considering the specificities of *in vivo* Dentistry applications.

The main motivation for the use of this computational resource is twofold: the efficient spectra evaluation for outcome prediction with a limited database and optimization of the configuration of the *in vivo* Raman spectrometer.

This network will be trained with Raman spectra obtained from enamel samples in different stages of induced demineralization: an in vitro protocol for the evaluation of the demineralization/remineralization of enamel will be developed and implemented at the Faculty of Dentistry using demineralizing acidic cycles and gold standard products for preventive Dentistry.

This way, we will develop an accurate assessment tool based on the prediction of the Raman spectra features, that translates into standardized diagnostic decision making and treatment evaluation in a future clinical setting. Moreover, we will be able to determine how early a diagnostic of demineralization can be achieved and until when remineralization therapies are efficient, setting grounds for major improvements in the preventive Dentistry industry.

Framework:

The 2016 Global Burden of Disease Study estimated that oral diseases affected half of the world's population and the most prevalent condition was dental caries in permanent teeth, an infectious microbiologic disease that results in the demineralization of dental tissues and formation of cavities. Conventionally, it was believed that the loss of mineral content in teeth was permanent but in recent decades a paradigm shift has been occurring in dental care where a more preventive and conservative approach is pursued. There are, nowadays, several products advocating restoration of lost mineral and/or strengthening of the hydroxyapatite lattice. For these products to be used efficiently, the diagnosis must occur as early as possible in the progression of the disease and should be as fast and accurate as possible. Raman spectroscopy could be that diagnostic technique, but the accuracy of the spectra evaluation must be improved. This thesis will set grounds for this improvement and successful *in vivo* application.

Calendarização das Tarefas:

The proposal is divided in 4 main tasks that will occur in concurrently:

<u>Task 1</u> (12 months) - Development of an erosive cycle for the creation of artificial carious lesions in human enamel - In this task, an *in vitro* erosive cycle, will be developed intending to simulate as closely as possible the real intraoral conditions. Specimens of sound enamel will be exposed to this erosive cycle and to remineralization cycles in order to create lesions with increased severity.

<u>Task 2</u> (12 months) – Raman spectra evaluation using function-based fitting - Specimen produced in task 1 will be evaluated using previously tested methodologies based on Raman analysis in LIBPhys-NOVA facilities, using existing benchtop Raman microscope. These methodologies are based on the evaluation of the symmetric stretching band of phosphate at ~ 959 cm-1 and the evaluation of its depolarization ratio, anisotropy, full width at half maximum (FWHM) and band center position.

<u>Task 3 (12 months)</u> - Spectra evaluation of XploRA spectra using Machine Learning algorithms - Data acquired in tasks 1 and 2 will be used as input to train the Machine Learning (ML) algorithm for Raman spectra evaluation. The input of the machine will be the spectra, with all its rich information, and the output will

approach the demineralization estimation made by the standard method of depolarization ratio determination using frequentist analysis. The expectation is that the developed system will be a more robust estimator, as it will not be prone to fatigue or subjective evaluation.

In addition to the aforementioned main goal, and because the overall project aims at producing a dedicated Raman spectrometer, we will search for the minimal set of input data, entering the ML predictor, that achieves a predictive power that is deemed sufficient for deployment of the technique. That will be performed in the design of the ML architectures to be tested, by pruning such structures, as well as by understanding the networks that are found to be successful in the prediction task.

Task 4 (18 months) – Benchmarking of the spectra evaluation tool using the *in vivo* Raman probe - combining the knowledge gained in previous tasks, an optimized version of the demineralization-remineralization protocol applied in task 1 and an adjusted CNN architecture developed in task 3 will be put to practice. A new set of samples will be created and treated but all samples will be used as input to train the ML algorithm.

Location:
FCT-NOVA, FMDUL

Candidate profile
Master Biomedical Engineering, Master Physics Engineering, Master Physics.

Orientador

- Nome: Sofia Pessanha
- Instituição: FCT-NOVA
- Email: sofia.pessanha@fct.unl.pt
- ORCID ID: 0000-0002-6039-2494

Co-Orientador

- Nome: Ricardo Vigário
- Instituição: FCT-NOVA
- Email: r.vigario@fct.unl.pt
- ORCID ID: 0000-0003-0950-6035

Co-Orientador

- Nome: João Silveira
- Instituição: FMDUL

- Email: joaosilveiramd@gmail.com
- ORCID ID: 0000-0001-9366-0662