Measurement Systems Engineering
Master thesis

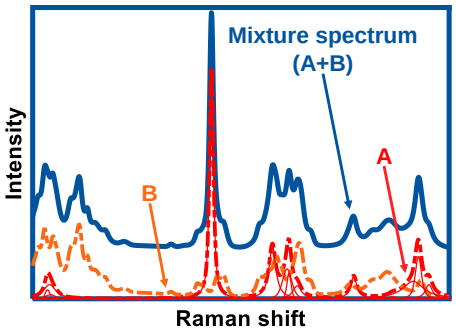
Automated selection of the optimal spectral range for the quantitative evaluation of Raman spectra with Indirect Hard Modeling (IHM)

Our Profile

The Institute of Technical Thermodynamics (LTT) of RWTH Aachen University, headed by Prof. Dr.-Ing. Niklas von der Aßen, deals with the analysis of thermodynamic systems on all size scales: from molecules to complete processes. One of the LTT's working groups is the Measurement Systems Engineering (OMT) group, which is an interdisciplinary team of young scientists working experimentally and theoretically. We are engaged in the development of non-invasive, very accurate, and highly efficient measurement methods as well as in the model-based, experimental determination of material data.

Background

Raman spectroscopy is a spectroscopic approach that analyzes the inelastic light scattering and allows to quantitatively analyze the composition of samples. Raman spectra are highly complex and their evaluation is challenging. A physics-based method for the evaluation of Raman spectra is Indirect Hard Modeling (IHM). In IHM, Raman spectra of mixtures are interpreted as weighted sums of the respective pure component spectra and the corresponding weighting factors are directly proportional to the concentrations of the mixture's components. As for every evaluation model, the spectral range used for analysis has a significant impact on the prediction quality. Therefore, the spectral range should be selected carefully for every system. Since manual testing of different spectral ranges is effortful and time-consuming, IHM's applicability and prediction quality could be improved by an algorithm that allows automatized selection of the optimal spectral range.



Task

In your master thesis, you will develop an algorithm that enables to automatically select the optimal spectral range for the quantitative evaluation of Raman spectra using IHM. For this purpose, we will provide you with several data sets from which we know that the selection of the spectral range significantly influences IHM's prediction quality. The algorithm's objective function will be to incrementally improve IHM's prediction quality for the respective dataset. The algorithm will be developed using MATLAB and must be combined with our in-house IHM script.

Your Profile

- You study Mechanical Engineering / Industrial Engineering / CES / Computer Science or a comparable course of study.
- You are interested in spectroscopy.
- You are interested in programming.
- You ideally already have some basic knowledge in the use of MATLAB.
- You are have an independent and goal-oriented way of working.

Our Offer

We offer you a versatile thesis, in which you will gain insights into various disciplines. You work in a motivated team and are in close, constant exchange with your supervisor, which gives you the opportunity to contribute and implement your own ideas. Your thesis can be written either in German or English.

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If you are interested, please contact:

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