Spectral Decomposition Methods for Coherent Raman Spectroscopy

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Spectral fidelity of any coherent Raman spectra is a major concern of building and/or using an instrument in "real-time" applications such as e.g. chemical component monitoring in a reaction chamber, or mapping the distribution of certain chemicals in a solid sample matrix. Mainly, three methods are used to recover the vibrational information from the measured spectra: 1. Nonlinear fitting based upon the Levenberg-Marquardt algorithm[1], 2. Maximum Entropy Method[2], and 3. Direct phase retrieval procedure based upon the assumption that the third order susceptibility is an analytic function[3].

Corrections for instrumental response and the problem of finite sampling with appropriate "windowing" are also necessary to recover the vibrational bands needed to identify or characterize the samples.

These mathematical methods will be explained and a computer program written in LabView will be presented. Spectra taken by a nanosecond (at UWF)[4] and a picosecond (at UofA)[5] CARS spectrometer will be presented and analyzed by all three methods, vice infra. It is concluded that the third method is the most appropriate one for "real-time" data processing.

References:

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