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Correlation analysis of spectroscopic data

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ABSTRACT

A method of correlation analysis of spectroscopic data is developed that allows the determination of patterns in experimental results with and without the application of a functional physico-mathematical model. In the latter case the method of correlation analysis allows to determine the regression values that occur in a physico-mathematical model. The method is applicable if the result of an experiment is the relationship between one physical variable and two or more parameters. The key idea of the method is search for particular measuring ranges of one of the parameters, where functional relationships of the physical value and one of the other parameters are either similar to each other or similar to some theoretical relationship. The ranges are found using the maximum of the cosines between two experimental data vectors or between the experimental data vector and the functional physico-mathematical model vector. The concept of a correlation spectrum that plays the major part in the correlation analysis of the experimental relationships between physical values and length or frequency of waves is introduced. The possibilities of the method are illustrated using the correlation analysis of the up-converted luminescence spectra of the YF_3:Yb^{3+} (20 at.%), Tm^{3+}(1 at.%) crystal that were captured at 13 equidistant power values of a laser diode stationary emission: $P \in (P_{min}, P_{max})$, $P_{min} = 253.3$ mW, $P_{max} = 1108$ mW, $\lambda_{ex} = 934$ nm. Using the correlation spectra a strong correlational relationship is determined between $^3P_2$ and $^1D_2$ energy levels populations of the Tm^{3+} ion as well as weak spectrum line of $Tm^{3+}(^3P_2 \rightarrow {}^1D_2)$ that is not visible in a regular luminescence spectrum was determined. The properties of the correlation spectrum allows to assert that this line is determined by stimulated emission.

1. Introduction

The goal of a spectroscopic experiment is the determination of patterns in the interaction of electromagnetic radiation and matter, and also patterns in the interaction of separate parts of the matter. In order to achieve this goal functional physico-mathematical models that are created to describe the interactions are usually experimentally tested. That said the necessity to change experimental conditions emerges. For example, in the optical spectroscopy temperature, chemical composition of the studied object, wavelength and emission intensity as well as type of the emission modulation (pulse, rectangular, sinusoidal) and time properties of the modulation (pulses duration and period, phase) are changed most frequently. Often, several experimental conditions vary simultaneously. All this makes spectroscopic experiments complicated and expensive.

Results of a spectroscopic experiment are presented as arrays of numerical data that represent relationships between certain physical values (luminescence/absorption intensity, index of refraction, reflection coefficient, etc.) and other values (wavelength, time, pumping intensity, temperature, impurity concentration, etc.). Currently the most efficient and mathematically strict method of experimental data processing in spectroscopy is regression analysis: determination of functional physico-mathematical model parameters using a set of numerical data. However, the more precisely the functional physico-mathematical model describes an experiment the more parameters it includes and it is more difficult to conduct regression analysis. Apart from this, an increased number of model parameters requires enhanced precision and accuracy of the spectroscopic results. This may require precise and expensive equipment. But even if this equipment is used, interpretation of the spectroscopic experiment using regression analysis can be quite ambiguous. This leads to additional and often more complicated experimental research.

At the same time it is possible to determine patterns in spectroscopic experiment results without regression analysis, without further research and even without functional physico-mathematical model. For example, in order to determine energy emission and absorption process which is a key factor to energy levels

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