Evaluation of the nanoscale spectroscopic and chemical mapping results of carbon nanotube composite materials

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INTRODUCTION

Modern technique combining infra-red spectroscopy and atomic force microscopy (AFM) allows the chemical mapping with the spatial resolution down to 30 nm. However, due to the specific detection of the infrared signal, special attention must be paid to data-processing stage. In this contribution evaluation of the nanoscale chemical mapping results of carbon nanotube composite materials will be presented. Nanostructural composites reinforced with carbon nanotube assemblies, such as CNT fibres or mats are promising materials for the numerous applications from avionics to high-tech industry [1]. Ability to gain insight into the chemical composition of such composite materials may provide a way for their further improvement.

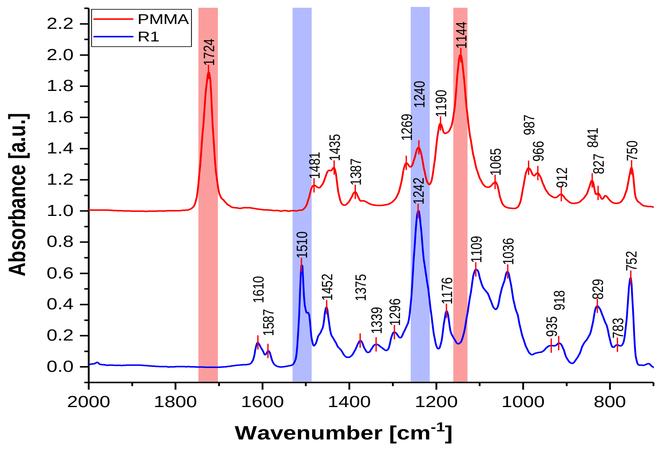
SAMPLES, DATA and METHODS

The CNT fibre nanocomposites were analyzed by means of nanoIR2 system (Anasys Instruments, USA). The obtained results were carefully evaluated with the help of open source software suites: R environment [2-5], ImageJ [6] and Gwydion [7] in order to ensure interpretability and reproducibility of the subsequent data.

BIG DATA

- matrix size 400 by 100 pixels^2
- n IR bands measured
- data frame with 6 times n variables and 40000 observations
- Big Data algorithms required for:
  - feature selection
  - clustering
  - dimension reduction

REFERENCE SPECTRA



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[2] R Core Team. R: A Language and Environment for Statistical Computing, 2017. URL `http://www.r-project.org/`.

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[5] Sébastien Lê, Julie Josse, and François Husson. FactoMineR: A package for multivariate analysis. *Journal of Statistical Software*, 25 (1):1–18, 2008. doi: 10.18637/jss.v025.i01.

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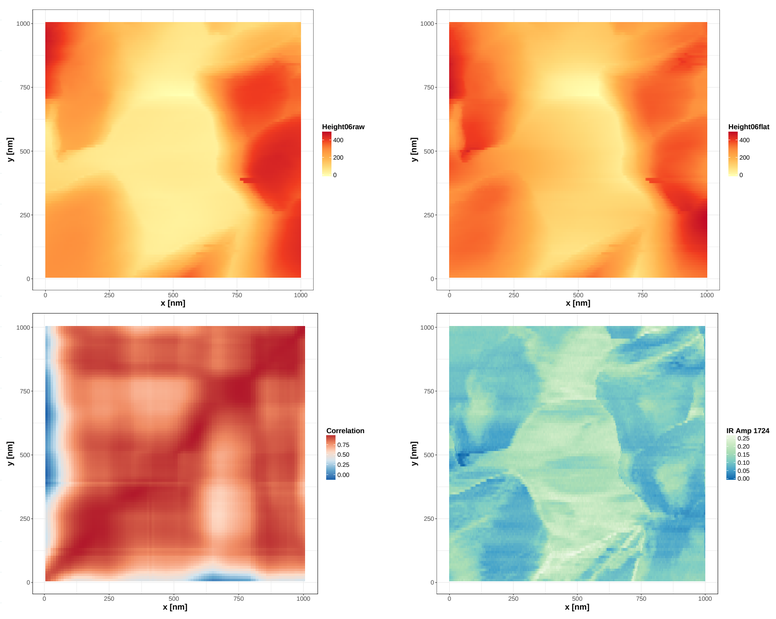
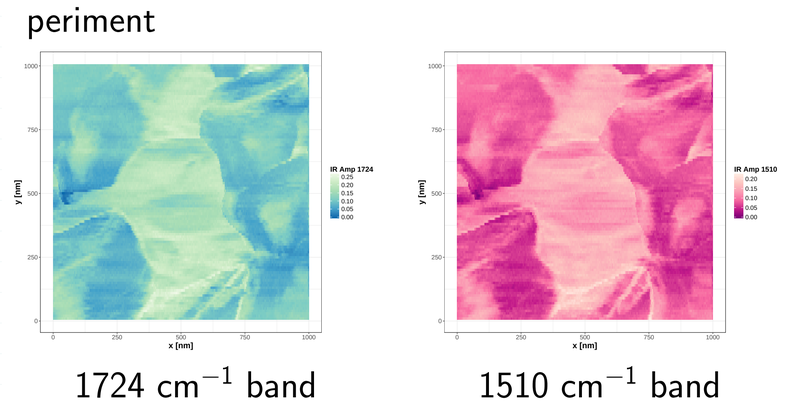
MAPS PRE-PROCESSING

Experimental data pre-processing includes image flattening and correlation for thermal drift.



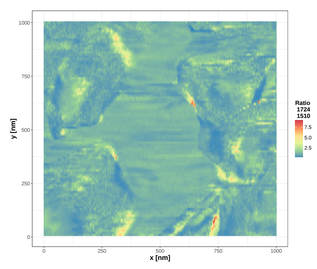
INFRA-RED MAPPING

2D maps for various IR bands recorded during experiment

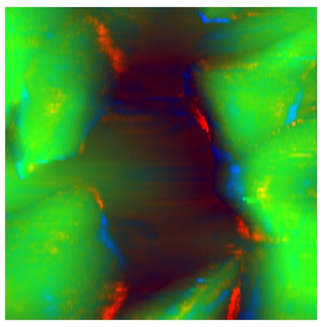


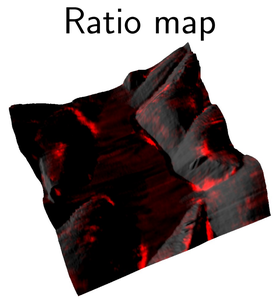
RATIOS and RGB COMPOSITE MAPS

Map of 1724/1510 cm^{-1} ratio imposed on topography image in surface plot and RGB representation.

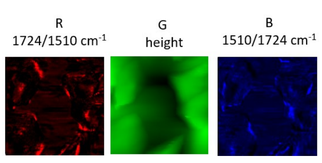


Ratio map





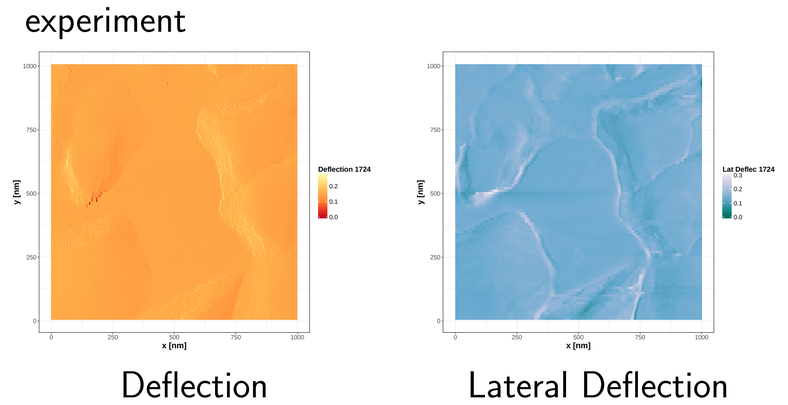
Surface plot with the ratio as the texture



RGB composite image

STRUCTURAL and IR VARIABLES

2D maps for structural parameters recorded during experiment



CONCLUSIONS

- combined infra-red spectroscopy and atomic force microscopy is a technique allowing to assess the chemical diversity of the sample with the spatial resolution down to 30 nm
- recorded amount of data required special approach for pre-processing and analysis of the results to retrieve essential information
- R Environment with its capability to use Big Data algorithms together with high-quality graphics and reproducibility (due to code-driven analysis) is a perfect solution for processing of AFM-IR experimental results

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