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SpectraFox: A free open-source data management and analysis tool for scanning probe microscopy and spectroscopy

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Abstract

In the last decades scanning probe microscopy and spectroscopy have become well-established tools in nanotechnology and surface science. This opened the market for many commercial manufacturers, each with different hardware and software standards. Besides the advantage of a wide variety of available hardware, the diversity may software-wise complicate the data exchange between scientists, and the data analysis for groups working with hardware developed by different manufacturers. Not only the file format differs between manufacturers, but also the data often requires further numerical treatment before publication. SpectraFox is an open-source and independent tool which manages, processes, and evaluates scanning probe spectroscopy and microscopy data. It aims at simplifying the documentation in parallel to measurement, and it provides solid evaluation tools for a large number of data.

Keywords: Scanning probe microscopy; Scanning probe spectroscopy; Data overview; Data management; Data analysis; Batch processing

Code metadata

Current code version	2016.04.01.0
Permanent link to code/repository used of this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-16-00022
Legal Code License	LGPLv3.0
Code versioning system used	git
Software code languages, tools, and services used	VB.NET, C#
Compilation requirements, operating environments & dependencies	.NET Framework 4.5
If available Link to developer documentation/manual	http://wiki.spectrafox.com
Support email for questions	contact@spectrafox.com

Software metadata

Current software version	2016.04.01.0
Permanent link to executables of this version	https://github.com/ElsevierSoftwareX/SOFTX-D-16-00022
Legal Software License	LGPLv3.0
Computing platform/Operating System	Microsoft Windows Vista or higher (32- or 64-bit)
Installation requirements & dependencies	.NET Framework 4.5, data acquisition tools: SPECS/Nanonis, Omicron/Matrix, Createc, Nanotec/WSxM
If available, link to user manual—if formally published include a reference to the publication in the reference list	http://wiki.spectrafox.com
Support email for questions	contact@spectrafox.com

E-mail address: m@mikeruby.net.

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1. Motivation and significance

Scanning probe microscopy and spectroscopy has become one of the key technologies in modern surface science. This is due to its capabilities in real space investigation of surface structures and their local electronic or magnetic environment. The technique has forked into many different variations, which specialized to different fields of research [1–6]. They all have in common that a sharp probe, for instance the apex of a metal wire, scans the sample surface in close vicinity. The measured quantity reveals the interaction between tip and sample, which may be, e.g., an electric current in scanning tunneling microscopy, or a force in atomic force microscopy.

Independent of the exact operation principle of the microscope, two types of data can be generated. In scanning probe *microscopy* (SPM) the output is a two-dimensional matrix of values representing the spatial variation of a specific sample parameter. The most prominent example is the surface topography. In scanning probe *spectroscopy* (SPS) the output is a one-dimensional trace of values, which is recorded at a single spatial location, where the reaction of the sample is measured on the variation of a junction parameter. For instance, in scanning tunneling spectroscopy the sample bias voltage is changed to measure the differential conductance of the junction.

Many independent research laboratories and manufacturers have improved SPM and SPS in the last decades. This includes the construction of different data acquisition systems, of which most of them use a proprietary file format to store their data. This complicates the exchange between scientists. It is especially problematic for research groups dealing with hardware from different manufacturers. The quality of the data analysis tools provided by the hardware suppliers also differs in their quality and features. So far only two free tools address these issues [7,8]. Only one of them is available under terms of an open-source license. The focus of these programs lies in handling microscopy images, rather than spectroscopy files.

SpectraFox is a free, independent, and open-source data management and analysis tool, which closes this gap, and puts a focus on the handling of spectroscopy files. It is suited to accompany a project during an ongoing measurement to keep the overview of the measured data, and to extract data quickly for documentation. After the measurement, SpectraFox provides tools for elaborated data analysis and evaluation. It includes many features, such as simple numerical data treatments applicable to a whole batch of files, or more complex features, such as non-linear least square fitting, and advanced visualization techniques. Finally it can export all results, e.g., to formats used in commercial software, such as OriginLab's Origin, Wolfram's Mathematica or Mathworks Matlab, which may be used to create a publication-ready output.

Since its launch, SpectraFox has proven its capabilities in the daily work of several research groups, and contributed to multiple publications [9–13]. This article describes the main features of SpectraFox. It extends the detailed instruction manual available online. We demonstrate its capabilities in a real world example, where we show the evaluation of a set of physical data recorded with a low-temperature scanning tunneling microscope under ultra-high vacuum conditions.

2. Software framework

2.1. Software architecture

SpectraFox is based on Microsoft's .NET Framework 4.5. Its user interface is based on multiple windows for each functionality. Multi-threading is heavily used, which takes advantage of modern multi-core processors. For complex numerical problems the computation capabilities can be further improved by using a dedicated graphic processor via the OpenCL or CUDA interfaces.

The software is released under an open-source license and features a plugin-interface. Both allow an easy extension of the software's capabilities by the user, such as custom file handling routines, data treatment procedures, or models for the non-linear least square fitting.

SpectraFox's architecture is sketched in Fig. 1. It manages data files by dedicated project folders. The typical usage scenario is to point the software to the folder containing the output of a manufacturer's measurement software. SpectraFox scans the directory for compatible files, and creates an index which is stored in a cache-file. This index contains measurement related information included in the file-headers, and allows to search for data with specific properties. As scanning all files may be a heavy task for projects containing many thousand files, the usage of a cache-file speeds up subsequent loading times. For larger projects, this architecture retains a low memory footprint.

The output generated by SpectraFox's data treatment routines is stored separately from each source file. This always keeps the original data untouched. It protects from data corruption, thus forbidding any manipulation of scientific data.

2.2. Software functionalities

SpectraFox is a tool that collects and displays measurement related meta-information extracted from the headers of the data files. For instance, the user comments, the record location of spectra or images, the record time, or the junction properties, such as feedback conditions or voltages. This collection of information is displayed in an overview for all data-files, together with preview images of the data itself. The list is sortable, and can be filtered or searched for files with specific properties. Furthermore, SpectraFox does not treat spectroscopy data separated from microscopy images. Instead it connects spectra recorded at different locations of the sample with related images.

A primary goal of SpectraFox is to simplify the processing of a large number of data-files. Therefore all basic operations applied to spectroscopy files are applicable not only to one file, but can be executed, once set up, to many files simultaneously. These basic tasks for spectroscopy data comprise

1. offsetting data columns, or adding multiple columns,
2. multiplying data columns with a scalar factor or values of another column,

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