Technical and Software Improvements of the EPR Spectroscopy Station at the NovoFEL Facility: Status 2020

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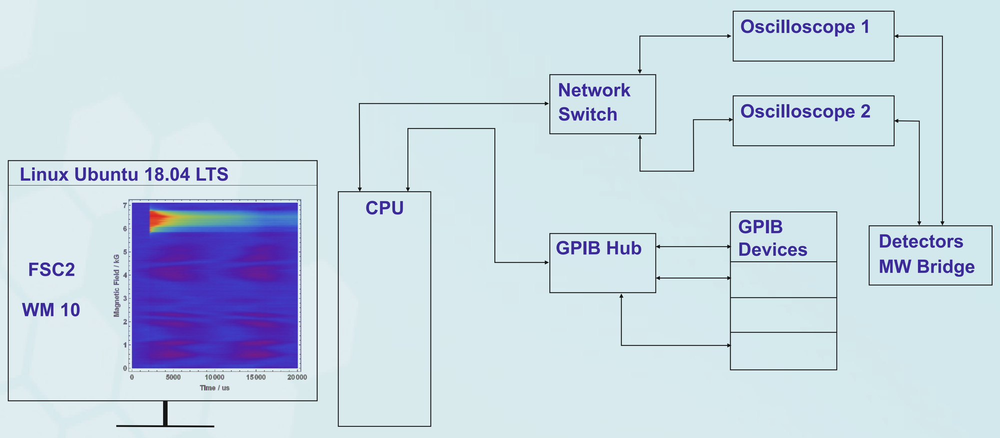
Abstract

The X-band Electronic Paramagnetic Resonance (EPR) spectroscopy station at the Novosibirsk Free Electron Laser (NovoFEL) facility is capable for steady-state (CW) EPR and time-resolved (TR) continuous wave EPR experiments.

Recently several upgrades in experimental hardware and software were done, aiming to more productively spend the time of an experimental session and increase the control of experimental parameters during the session. Firstly, we installed several detectors with different time resolution for tracking radiation produced by NovoFEL. Secondly, on the basic of fsc2 program, we implemented a possibility of simultaneous use of two oscilloscopes, configured at different timescale or sensitivity. Finally, we developed special software for on-the-fly CW and TR experimental data viewing and treatment.

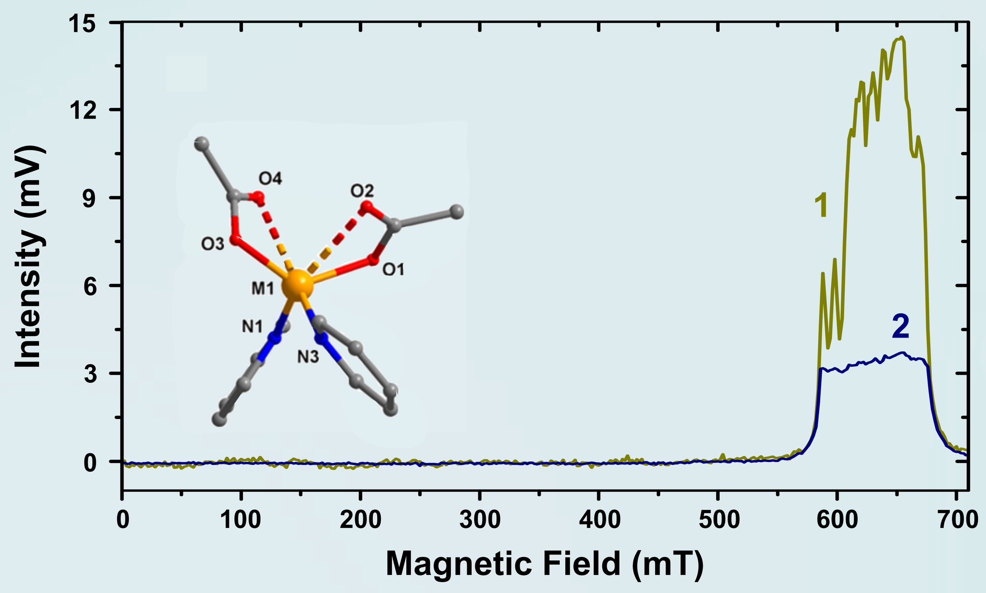
Hardware Improvements

I. The Use of Two Oscilloscopes

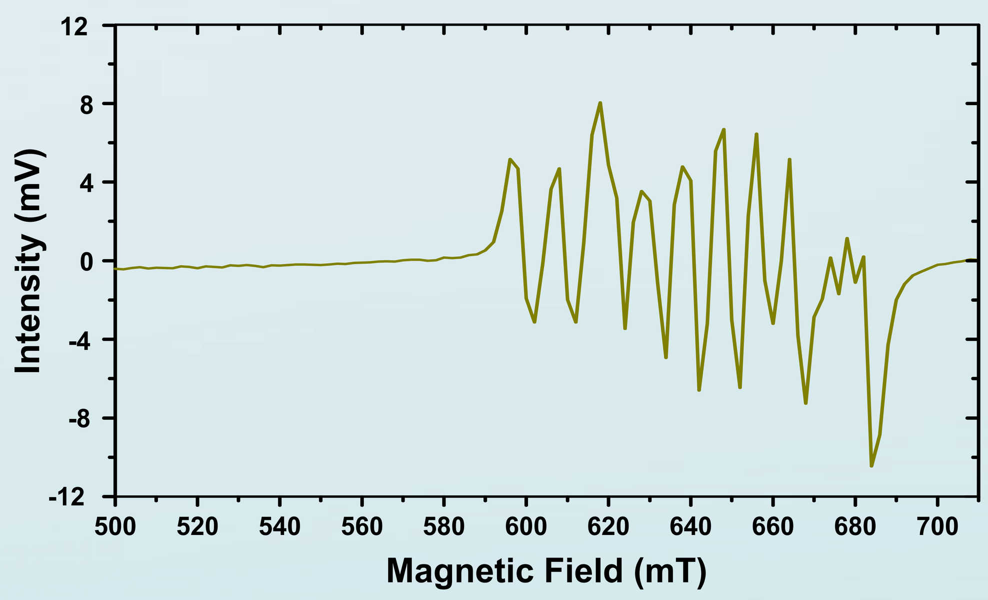


General scheme of the control computer with the network of ethernet and GPIB devices

To automatize measurements and have possibility to easy adapt to different hardware, an open-source fsc2 program (www.fsc2.org). This program employs modular approach to the handling of devices that allows using new devices by writing special modules for them in C programming language. To optimize the time distribution of an experimental session, it is possible to use two oscilloscopes simultaneously for detection signals with distinctive characteristic at the same time. It was realized using fsc2 for which a new module for Keysight oscilloscope was written.



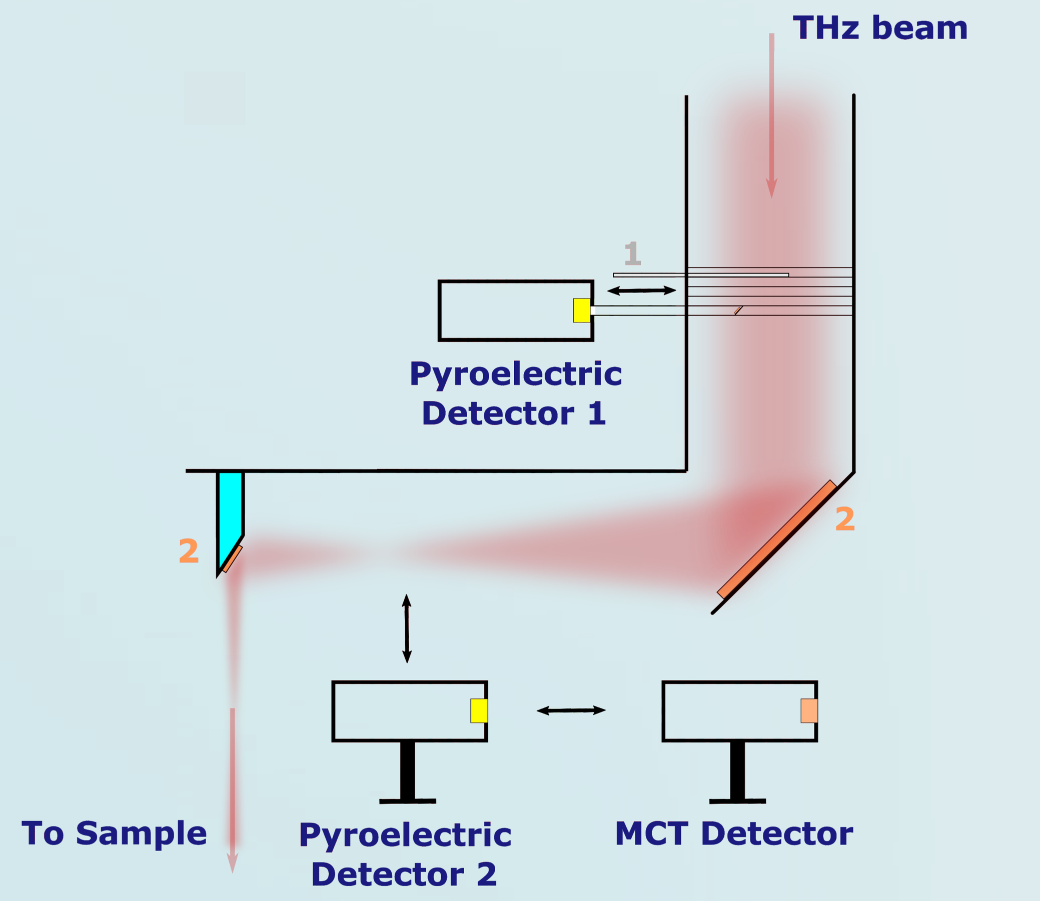
Cross-sections of TR EPR spectrum of $[Co_{0.01}Zn_{0.99}(piv)_2(2\text{-}NH_2\text{-}Py)_2]$ right after THz macropulse measured simultaneously at two oscilloscopes with different sensitivity: **1** – 500 mV, **2** – 30 mV. Temperature is 4.7 K, microwave frequency is 9.76 GHz, microwave power is 2 mW, THz radiation pulse length is 100 μs, repetition rate is 10 Hz, wavelength is 41.7 cm^{-1}. The inset shows structural formula of $[Co(piv)_2(2\text{-}NH_2\text{-}Py)_2]$. Methyl groups in pivalate and amino group in 2-aminopyridine are omitted for clarity



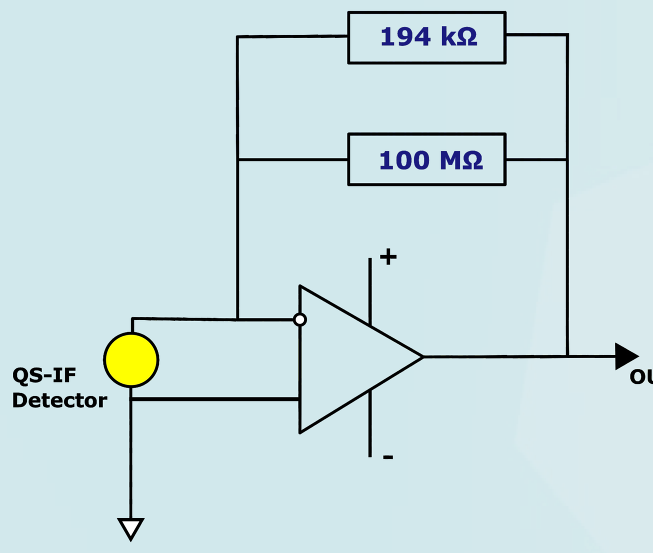
CW EPR spectrum of $[Co_{0.01}Zn_{0.99}(piv)_2(2\text{-}NH_2\text{-}Py)_2]$ measured at 5.3 K. MW frequency is 9.76 GHz, MW power is 20 μW, modulation amplitude is 0.3 mT, modulation frequency is 100 kHz, time constant is 30 ms

II. Detectors for THz Radiation

Controlling the shape and duration of THz macropulse during experiments is crucial for measuring TR EPR spectrum under THz radiation. At the moment the EPR spectroscopy station has three available THz detectors with different sensitivity and time resolution.

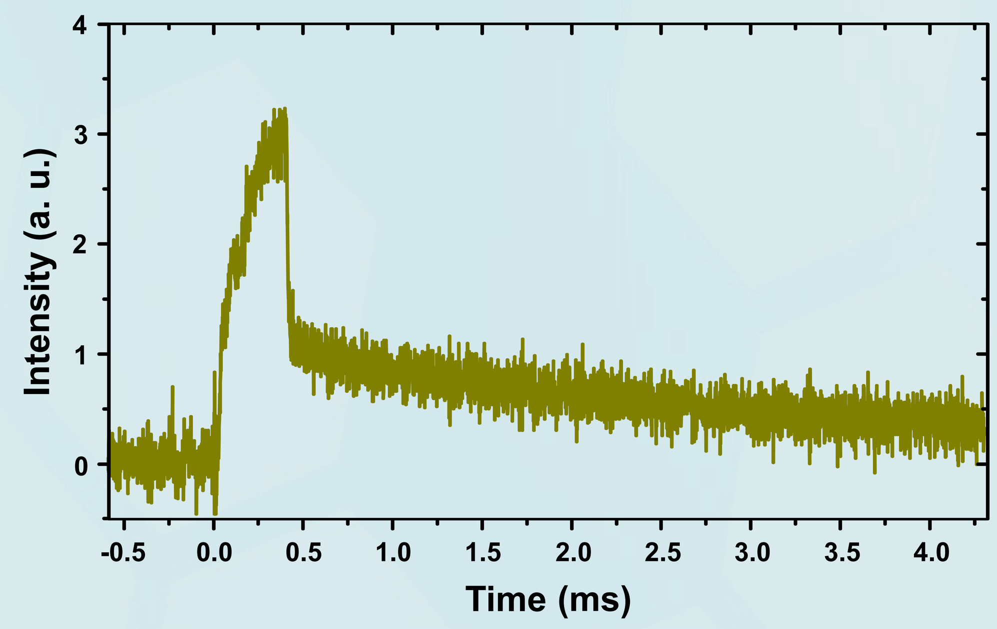


Layout of various THz detectors at the EPR spectroscopy station. Numbers show: 1 – movable mechanical shutter; 2 – off-axis parabolic mirrors. Detectors can be placed directly at the focus of the first mirror (pyroelectric detector 2 or MCT detector) or used to control the duration of THz macropulses during experiment (pyroelectric detector 1)

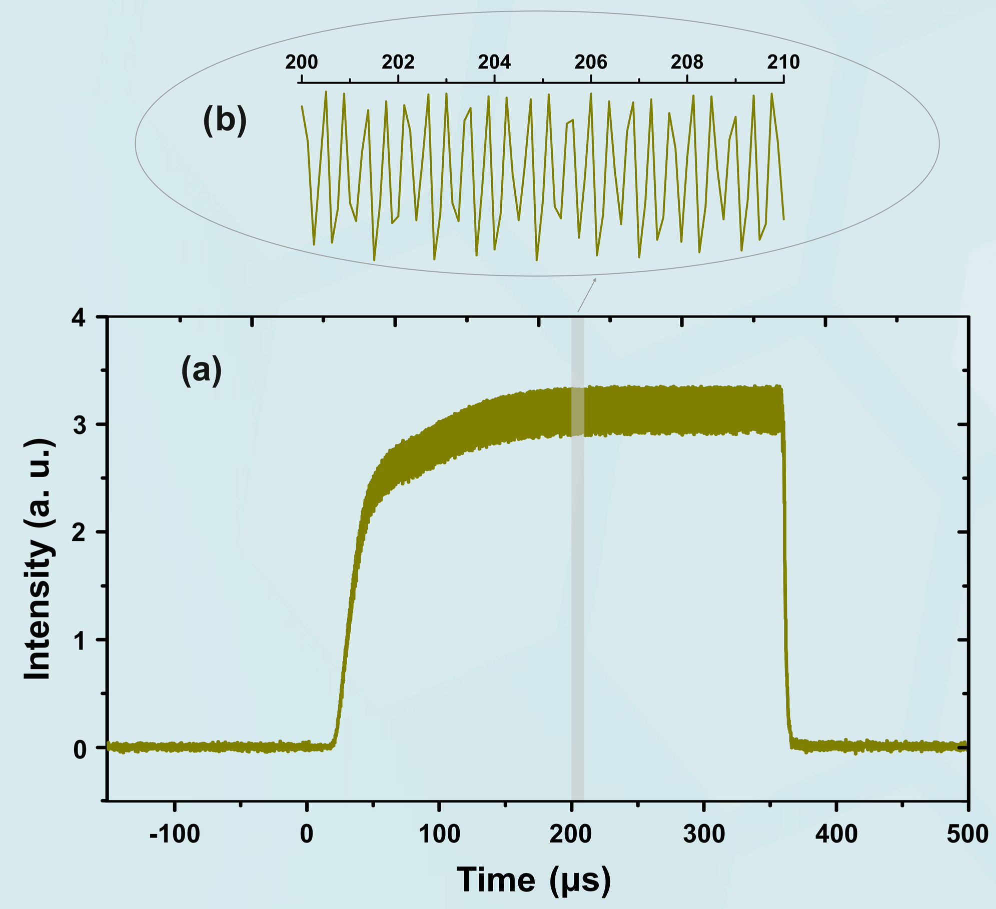


Circuit diagram of pyroelectric detector 2 with modified feedback resistor to improve time resolution

Pyroelectric detectors have a wide spectral sensitivity and can be used for all three FELs available at NovoFEL facility. In addition to them, MCT LN2 detector can be used in the mid-IR frequency range.



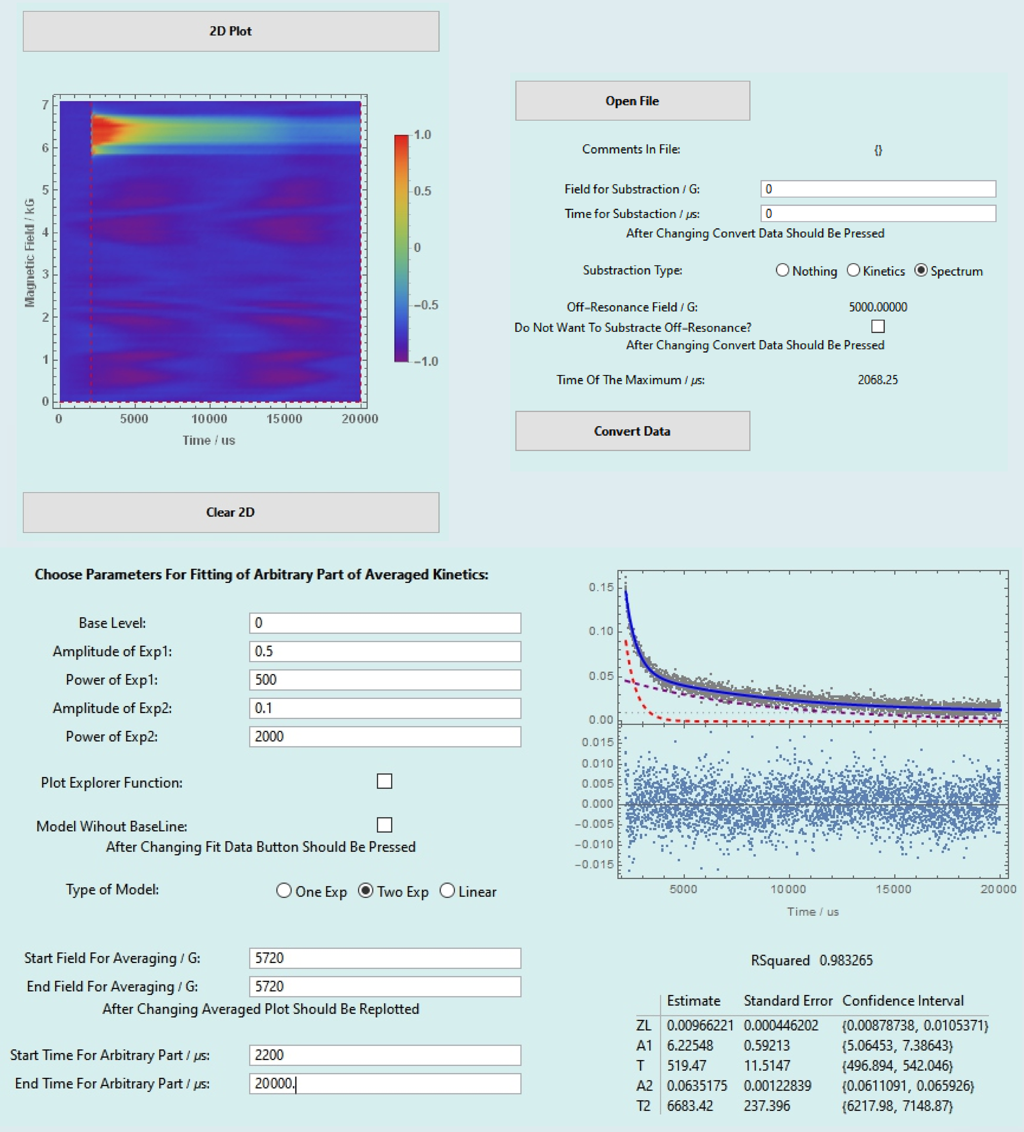
Example of THz macropulse with 400 μs duration registered by pyroelectric detector 1 at 76.9 cm^{-1}



(a) 350 μs THz macropulse registered by pyroelectric detector 2, (b) A closer view of **a** in the range of 10 μs with visible fine structure of the macropulse (limited by time resolution of the detector)

Software Improvements

Fsc2 is a versatile and flexible program for controlling spectrometers with a good graphical user interface that allows visualizing raw 2D and 1D data during experiment. At the moment, in this program there is no way to open previously saved data, since the user himself determines the format of it. The possibility of opening saved data directly on spectrometer for on-the-fly treatment and comparison is useful for any experimental technique, but it is especially important at large scale facilities where experimental time is limited. At the EPR spectroscopy station this possibility was realized using Wolfram Mathematica. At the core of the program lies the concept of dynamic visualization using Manipulators and Dynamic Modules of Wolfram Language.



Examples of graphical interface of WM program for experimental data visualization and treatment that is used at the EPR spectroscopy station at NovoFEL

Currently the program enables a number of basic manipulations with raw experimental data, such as baseline correction, normalization, plotting, etc. Plotting functions include 1D magnetic field and time cross-sections of time-resolved EPR spectrum with the possibility of averaging in the desired time or magnetic field range, and 2D density plot. Least squares fitting is available in an arbitrary chosen timespan using one or two exponential function as a model. All functions are realized using simple GUI.

Conclusions

In this work, we describe recent advances in experimental hardware and software at the X-band EPR station of the NovoFEL facility. There are three main improvements that help to optimize the time distribution of an experimental session and increase the control of experimental parameters during the session. The first upgrade is the implementation of three detectors with different time resolution and sensitivity that allows recording the THz macropulses during experiment. The second is the realization of the possibility of simultaneous use of two oscilloscopes, configured at different timescale or sensitivity. Finally, special software for CW and TR experimental data viewing and treatment was developed using Wolfram Mathematica. All the improvements allow spending experimental time more productively and carrying out experiments at a higher technical and software level.

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Thank You for Your Attention

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