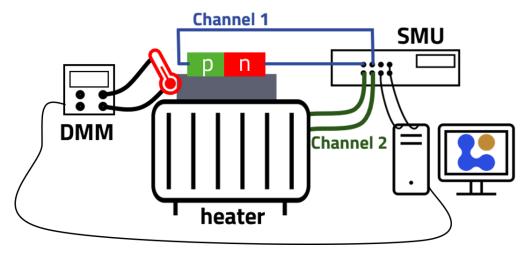


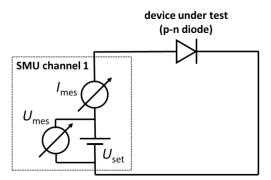
Controlling experiments and recording FAIR data with NOMAD CAMELS



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Exercise 1 (Simple I-V characteristics)

At first, we will only consider a simplified setup consisting of only the p-n-diode and the SMU. Measure the current-voltage (I-V) characteristics of a p-n diode using a source-measure unit (SMU).



Start CAMELS and enter basic metadata

- 1. Start NOMAD CAMELS. During the first start, you will be asked to define the data directory, into which the measurement data will be stored.
- 2. Enter the following metadata:
 - user name (add a new user and enter your name)
 - sample information (add new sample with
 - name: diode1,

sample_id: 12345

description: SandboxForCAMELS p-n diode

- give this **session** the name **DPG Hacky Hour**

Install and configure required instruments

3. Install the **demo_source_measure_unit** instrument driver from CAMELS' instrument manager. The **demo_source_measure_unit** is a 2-channel source-measure unit



connected to the experiment simulator SandboxForCAMELS. In the simulator, a p-n diode is connected to channel 1 of the **demo_source_measure_unit**.

 In the instrument manager, navigate to the tab Configure Instruments, and create an instance of demo_source_measure_unit with the name SMU. Keep all settings and leave the instrument manager by clicking OK.

Define the measurement protocol

- 5. Create a new measurement protocol. In the protocol sequence, add a step Simple Sweep. Configure the sweep channel to be SMU_setV1 (voltage of channel 1 of the SMU), the Start voltage as -10, the Stop voltage as 2, the number of data points 121. Read the following channels: SMU_mesI1 (current reading of SMU channel 1), SMU_mesV1 (voltage reading of SMU channel 1) and SMU_setV1 (voltage value set for SMU channel 1).
- On the simple sweep configuration page (right side), define a plot of type X-Y plot with the voltage SMU_mesV1 plotted on the x-axis, the current SMU_mesI1 on the y-axis.
 Hint: right click into the input boxes displays a context menu, from which you may choose the channel value. Enter meaningful title, x-label and y-label; use only letters and white spaces here.

Let's start the experiment

- 7. Close the protocol editor and start the measurement protocol.
- 8. Inspect the measurement data file. In order to view the nxs file (hdf5 format), you may use the h5web viewer available at https://h5web.panosc.eu/h5wasm.

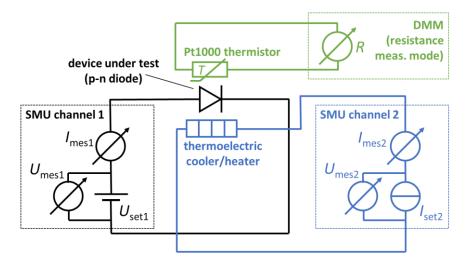
You can continue with Exercise 2 on the next page.

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Exercise 2 (Temperature-dependent measurement)

Measure the temperature-dependent I-V characteristics of a p-n diode. CAMELS provides a virtual experiment with a p-n diode mounted on top of a thermoelectric cooler/heater. The temperature is measured by a PT1000 thermistor mounted side-by-side with the p-n diode. The thermoelectric cooler/heater is connected to **Channel 2** of the SMU used in exercise 1, the Pt1000 resistance is measured by a digital multimeter (DMM) in resistance measurement mode. The p-n diode is connected to **Channel 1** of the SMU.



Install and configure required instruments

- Open the instrument manager and install the demo_digital_multimeter, and the PID instrument drivers. Go to the configure instruments tab and create an instance of demo_digital_multimeter with the name DMM.
- In the instrument manager add an instantiate of the PID controller. As input channel for the PID, configure DMM_resistance, as output channel SMU_setI2.
 Enter pt1000 as conversion function for reading.
 In the table of PID parameters, enter kp = 0.5, ki = 0.5, kd = 0.1

Define the temperature sweep

- 3. Edit the measurement protocol of exercise 1 as follows:
- Add a For Loop with name Temperature_sweep for the temperature sweep from 300
 K to 400 K with the following parameters: Start = 300, Stop = 400, # points = 6
- 5. In the loop, add a step Set Channels. Check set for the channels PID_pid_on and PID_setpoint and add the following values: PID_pid_on = 1, PID_setpoint = Temperature_sweep_Value (you may select this from the context menu, right click and Insert Variable). This activates the PID controller and sets the temperature setpoint to the current value of the For Loop.



- 6. After **Set Channels** in the sequence, insert a step **PID wait for stable**. The sequence will pause here, in order to wait for the temperature to be stable at the setpoint.
- 7. Move the **Simple Sweep** step into the loop as the last step (drag-and-drop). The I-V measurement will be executed for each temperature defined in the For Loop.
- Click onto the step Simple Sweep and check additionally PID_current_value and PID_setpoint in the Read-Channels list. This ensures that we store the temperature data along with the I-V data.

Stop the PID controller at the end of the measurement

Add a Set Channels step below the loop (not inside!).
 Set the channel PID_pid_on to 0 in order to switch off the PID controller at the end of the measurement protocol.

Let's start the experiment

- 9. Close the protocol editor by clicking **OK** and run the measurement protocol.
- 10. Inspect the measurement data file. To view the nxs file (hdf5 format), you may use the h5web viewer available at https://h5web.panosc.eu/h5wasm.

You can continue with Exercise 3 on the next page.



Exercise 3 (Automatic upload of measurement data into Electronic Lab Notebooks)

NOMAD CAMELS can directly upload the measurement data into your Electronic Lab Notebook (ELN). Currently, two open-source ELN applications are supported: NOMAD (Oasis) and eLabFTW. In this exercise, the workflow with NOMAD is demonstrated.



Some preparation

- Open NOMAD in your web browser via the link <u>https://nomad-lab.eu/prod/v1/staging/</u> and login. If you don't have a NOMAD user account, you can create one by clicking on Login / Register and then on Register at the bottom of the login form.
- 2. After login, create a new data space for your measurement data as follows: select Uploads from the top Publish menu. Then click Create a new upload. Give the upload the name Hacky Hour by clicking onto the pencil symbol next to unnamed upload. Don't forget to click Save.

Tell CAMELS to upload the measurement data to NOMAD

- 3. Back in the main window of CAMELS, select **NOMAD user** from the dropdown list in the user metadata section and click the button **NOMAD login**.
- 4. In the login window that is showing up, make sure that authentication type is **token** and **central NOMAD** is selected. Click the button **get the token!**. You will be redirected to a NOMAD webpage in your web browser. On this webpage, click onto the clipboard icon in the paragraph **App token**. This will generate and copy to clipboard a new app token that is valid only for today. Close the browser tab and go back to the login window of CAMELS. Paste the app token from the clipboard into the textbox **Authentication token**.

Click **OK**. CAMELS is now connected to your user space in NOMAD. Your user data (e.g. name) is automatically fetched from NOMAD and displayed on CAMELS' main window.

5. On the main window of CAMELS, select **auto upload** from the dropdown list next to **NOMAD Upload:**.

A second dropdown list will show up, which lists all your data spaces (uploads) on the NOMAD server, including the one ("Hacky Hour") we have just created in step 2; select it from the dropdown list.

Let's go and see

6. Start the measurement protocol of the previous exercise and watch CAMELS doing the measurements.



- 7. After the measurement is finished, go to NOMAD in your web browser and reload the upload **Hacky Hour**. You will find the measurement data file in the list of processed data.
- 8. Inspect the data by clicking the arrow (→) next to the entry. The interactive h5web viewer will show up within NOMAD.

Optional exercise 4 (Evaluation of data)

The I-V characteristics of the p-n diode is described by the Shockley equation

$$I = I_S(T) \left[\exp\left(\frac{e \cdot (V - R_S I)}{nk_B T}\right) - 1 \right]$$

with current I, voltage V, temperature T, electron charge e, Boltzmann constant k_B and the device parameters of the p-n diode: the ideality factor n, the series resistance R_S and the temperature-dependent saturation current $I_S \propto \exp\left(-\frac{E_{gap}}{k_BT}\right)$ with E_{gap} being the bandgap energy of the semiconductor.

Determine R_S , n and E_{gap} from the measurement data.

If you want to use Jupyter for the evaluation, you can start a Jupyter notebook directly in NOMAD (from menu Analyze, NOMAD remote tools hub) with access to your measurement data stored in NOMAD.

Download our example evaluation notebook from <u>here</u>.



Further information

Installation of NOMAD CAMELS

The full installation documentation is available at: https://fau-lap.github.io/NOMAD-CAMELS/doc/installation/installation.html

For Windows computers, you can download our installer, which automatically installs NOMAD CAMELS within a few minutes. The installer is available from: https://app.lap.nat.fau.de/nomad-camels/NOMAD-CAMELS_installer.exe

Contact and information

More information? Visit our documentation! <u>https://fau-lap.github.io/NOMAD-CAMELS/</u>

Questions?

- Join the discussions: <u>https://github.com/FAU-LAP/NOMAD-CAMELS/discussions</u>
- Or contact us directly: <u>lap-nomad-camels@fau.de</u>

Found a bug? Please report it! <u>https://github.com/FAU-LAP/NOMAD-CAMELS/issues</u>

NOMAD CAMELS is being developed at the Friedrich-Alexander-Universität Erlangen-Nürnberg within the FAIRmat NFDI consortium.

Chair of Applied Physics at FAU: <u>https://www.lap.physik.nat.fau.eu</u> FAIRmat: <u>https://www.fairmat-nfdi.eu/fairmat/</u>

Learn more about the NOMAD software family: <u>https://nomad-lab.eu/nomad-lab/</u>