

Supporting Information

High Precision Nail-Penetration Setup for the Controlled Thermal Runaway Initiation of Lithium-Ion Cells at Very Low Temperatures

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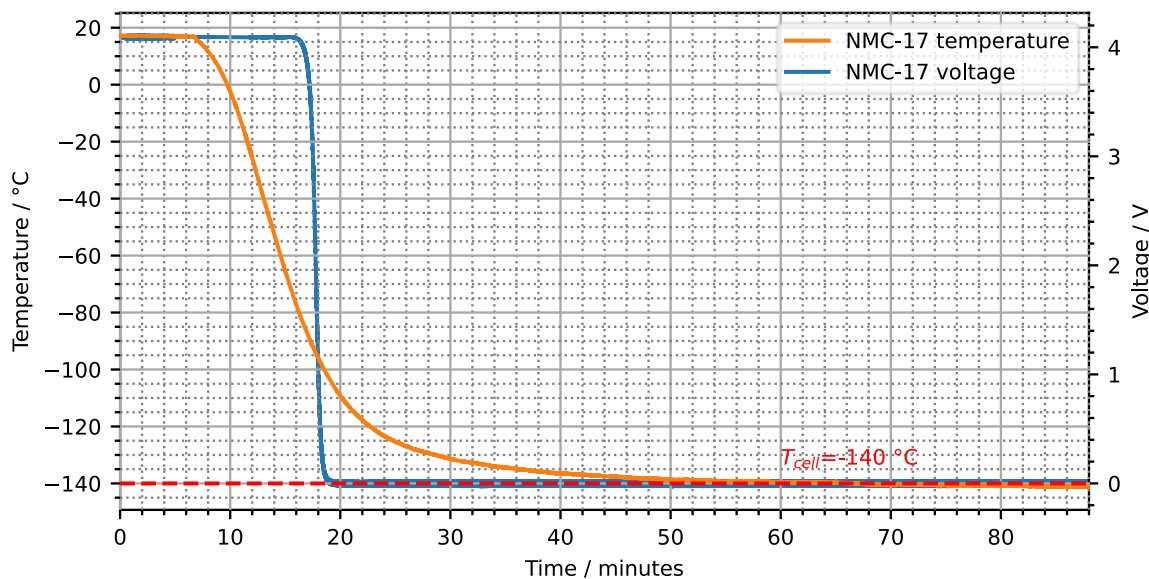


Figure S1: Exemplary cool-down process of an LIB-18650 cell inside the developed nail penetration set-up, utilizing the N₂-cold gas system (N₂-flow was set to -190°C).

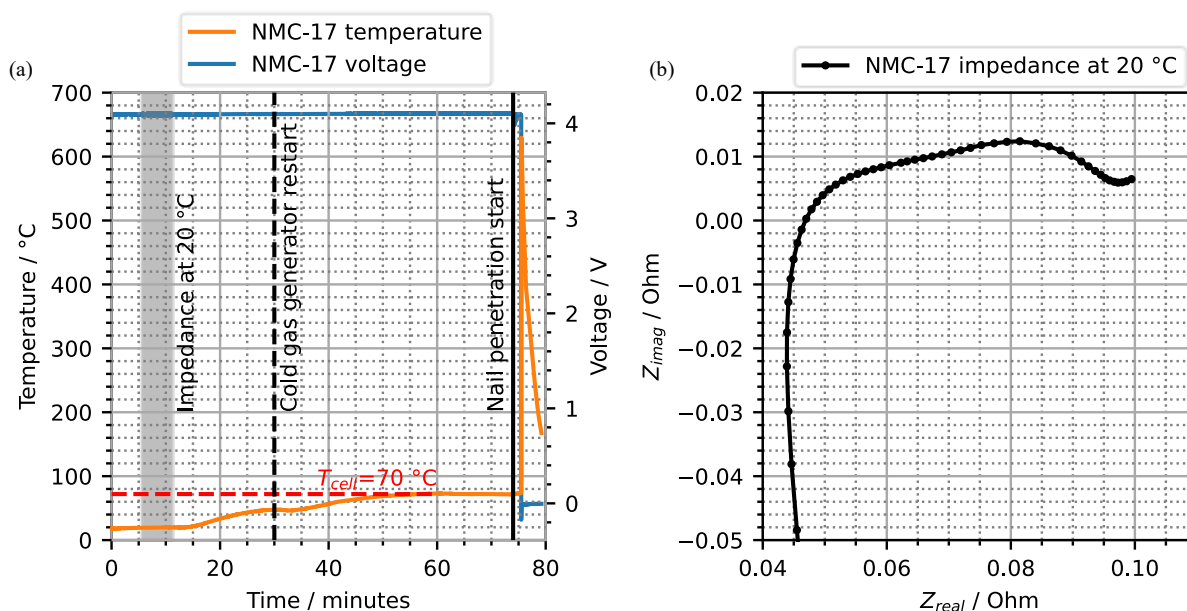


Figure S2: (a) Exemplary heating process of an 18650 LIB-cell inside the developed nail penetration set-up utilizing the N₂-cold gas system. First, the cell was kept at a controlled temperature of 20°C. At this stage, an EIS-measurement was performed. The cell was further heated with the N₂-flow, reaching a stable cell temperature of 70°C. Furthermore, a NPT was performed at this temperature. (b) Nyquist-plot of the corresponding EIS-measurement.

Table S1: Overview of all tests including the main test parameters.

| Cell type | Number | SOC | NPT temp. | Temp. control | NPT speed | NPT depth | Figure |
|-----------|---------|-----|----------------|-----------------|-----------------------|-----------|-----------------------|
| - | - | [%] | [°C] | - | [mm s ⁻¹] | [mm] | - |
| LFP | 1 | 0 | 17.5 | none | ≈45 | ≈21 | 3a, 3b |
| LFP | 2 | 0 | 18.5 | none | ≈45 | ≈21 | 3a, 3b |
| NMC | 1 - 4 | 100 | 21.5 (+/- 0.5) | Cold gas | ≈0.01 | till TR | 3c, 3d, S4 |
| NMC | 5 | 0 | 21.8 | none | ≈5 | ≈5 | 4a, 4b, 4e, 4f, S5 |
| NMC | 6 | 0 | < -170.0 | LN ₂ | ≈5 | ≈5 | 4c, 4d, 4e, 4f, S5 |
| NMC | 7 - 10 | 100 | -85.0 (+/- 5) | Cold gas | ≈45 | ≈12 | 5a, 5b, S6 |
| NMC | 11 - 14 | 100 | -85.0 (+/- 5) | Cold gas | ≈5 | ≈6 | 5a, 5b, S6 |
| NMC | 15 - 16 | 100 | - | LN ₂ | ≈5 | ≈5 | 6b, 6c |
| NMC | 17 | 100 | 70 | Cold gas | ≈0.01 | Till TR | S1, S2 |
| NMC | 18-21 | 100 | 20 | Cold gas | ≈5 | ≈8 | S3 |

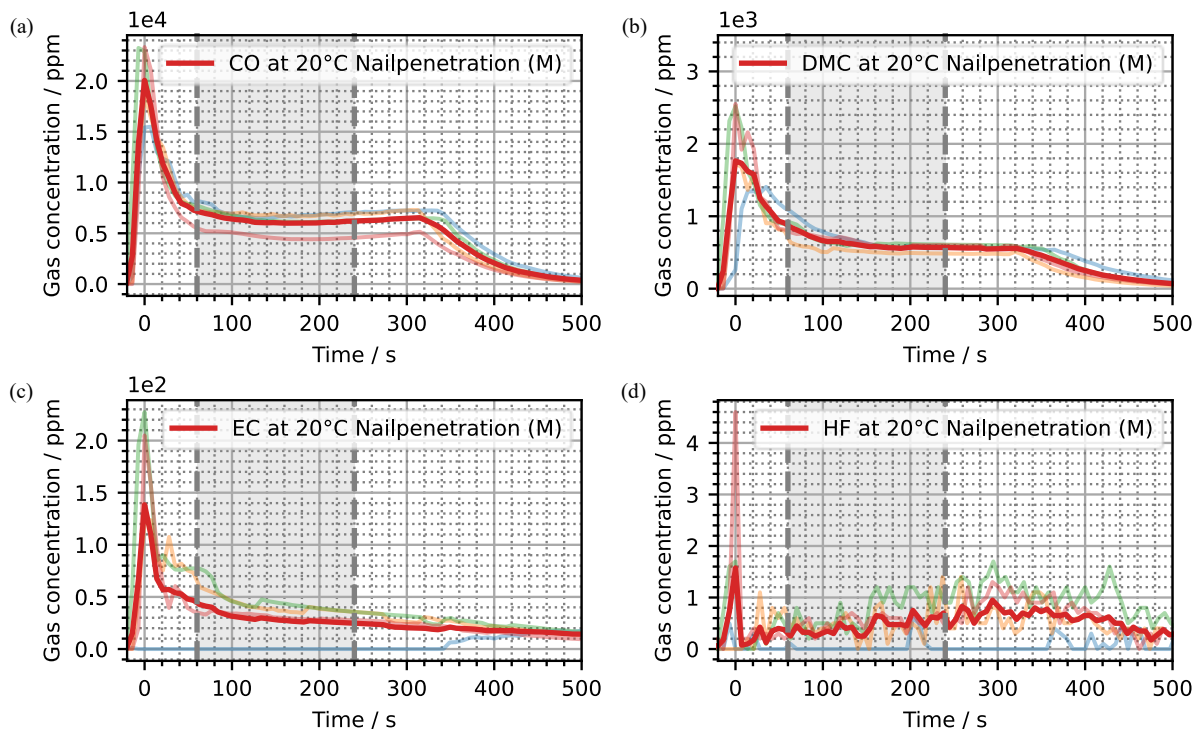


Figure S3: Exemplary time-resolved gas concentration of different LIB vent gases after the TR of an 18650 LIB-cell in the developed nail penetration set-up (NPT-parameters can be found Table S1). The data was recorded via FTIR which was operated in a closed loop (see also Figure 1a). The results of four typical species for LIB vent gases are shown, i.e., (a) carbon monoxide (CO), (b) dimethyl carbonate (DMC), (c) ethylene carbonate (EC) and (d) hydrogen fluoride (HF). The marked grey area represents the region from which the concentration of a certain gas species in the homogenized gas mixture after the TR can be calculated. The data was recorded from four test runs under the same conditions. The shown bold red graphs represent the main average (M) of the individual measurements. The selected FTIR method allows the simultaneous detection of various gas concentrations - possibly, each with a distinct order of magnitude - as denoted by the values specified at the top left of the respective graphs.

Table S2: Results of motion accuracy tests and overview of the selected boundary conditions.

| | Parameters | | | Full path | | | | Stepwise | | | | | |
|----------------|------------|------------|-----------------|----------------|---------------|-----------------|-----------------------|----------------|---|---|----------------------------|--|--|
| | Speed | Step width | Range | Mean deviation | Maximum error | Steps per range | Mean offset deviation | Mean Deviation | Minimum deviation of all steps regarding one test | Maximum deviation of all steps regarding one test | Maximum absolute deviation | Absolute difference between minimum and mean | Absolute difference between minimum and mean |
| Open loop | 5mm/s | 5mm | 0.5mm - 40.5mm | 0.04 | 0.09 | 8.00 | 0.01 | 0.01 | -0.03 | 0.05 | 0.08 | 0.04 | 0.04 |
| Open loop | 1mm/s | 5mm | 0.5mm - 40.5mm | 0.03 | 0.08 | 8.00 | 0.01 | 0.01 | -0.03 | 0.05 | 0.08 | 0.04 | 0.04 |
| Open loop | 5mm/s | 1mm | 0.5mm - 40.5mm | 0.07 | 0.16 | 40.00 | 0.00 | 0.00 | -0.02 | 0.03 | 0.05 | 0.02 | 0.03 |
| Open loop | 1mm/s | 1mm | 0.5mm - 40.5mm | 0.06 | 0.15 | 40.00 | 0.00 | 0.00 | -0.01 | 0.02 | 0.03 | 0.01 | 0.02 |
| Open loop | 2.5mm/s | 2.5mm | 20.5mm - 40.5mm | 0.06 | 0.09 | 8.00 | 0.01 | 0.01 | -0.03 | 0.03 | 0.06 | 0.04 | 0.02 |
| Closed loop EC | 5mm/s | 5mm | 0.5mm - 40.5mm | 0.11 | 0.20 | 8.00 | 0.02 | 0.03 | -0.01 | 0.07 | 0.08 | 0.04 | 0.05 |
| Closed loop EC | 1mm/s | 5mm | 0.5mm - 40.5mm | 0.02 | 0.07 | 8.00 | 0.01 | 0.00 | -0.07 | 0.06 | 0.13 | 0.07 | 0.06 |
| Closed loop EC | 5mm/s | 1mm | 0.5mm - 40.5mm | 0.36 | 0.71 | 40.00 | 0.02 | 0.02 | -0.01 | 0.04 | 0.05 | 0.03 | 0.02 |
| Closed loop EC | 1mm/s | 1mm | 0.5mm - 40.5mm | 0.09 | 0.13 | 40.00 | 0.00 | 0.00 | -0.06 | 0.03 | 0.09 | 0.06 | 0.03 |
| Closed loop EC | 2.5mm/s | 2.5mm | 20.5mm - 40.5mm | 0.11 | 0.17 | 8.00 | 0.02 | 0.02 | -0.02 | 0.05 | 0.07 | 0.04 | 0.03 |
| Closed loop LS | 5mm/s | 5mm | 0.5mm - 40.5mm | 0.11 | 0.19 | 8.00 | 0.02 | 0.02 | 0.02 | 0.03 | 0.03 | 0.00 | 0.01 |
| Closed loop LS | 1mm/s | 5mm | 0.5mm - 40.5mm | 0.06 | 0.11 | 8.00 | 0.01 | 0.01 | 0.01 | 0.02 | 0.02 | 0.00 | 0.01 |
| Closed loop LS | 5mm/s | 1mm | 0.5mm - 40.5mm | 0.56 | 1.07 | 40.00 | 0.03 | 0.03 | 0.02 | 0.04 | 0.04 | 0.01 | 0.01 |
| Closed loop LS | 1mm/s | 1mm | 0.5mm - 40.5mm | 0.21 | 0.44 | 40.00 | 0.01 | 0.01 | 0.00 | 0.02 | 0.02 | 0.01 | 0.01 |
| Closed loop LS | 2.5mm/s | 2.5mm | 20.5mm - 40.5mm | 0.08 | 0.14 | 8.00 | 0.02 | 0.02 | 0.01 | 0.02 | 0.02 | 0.01 | 0.00 |

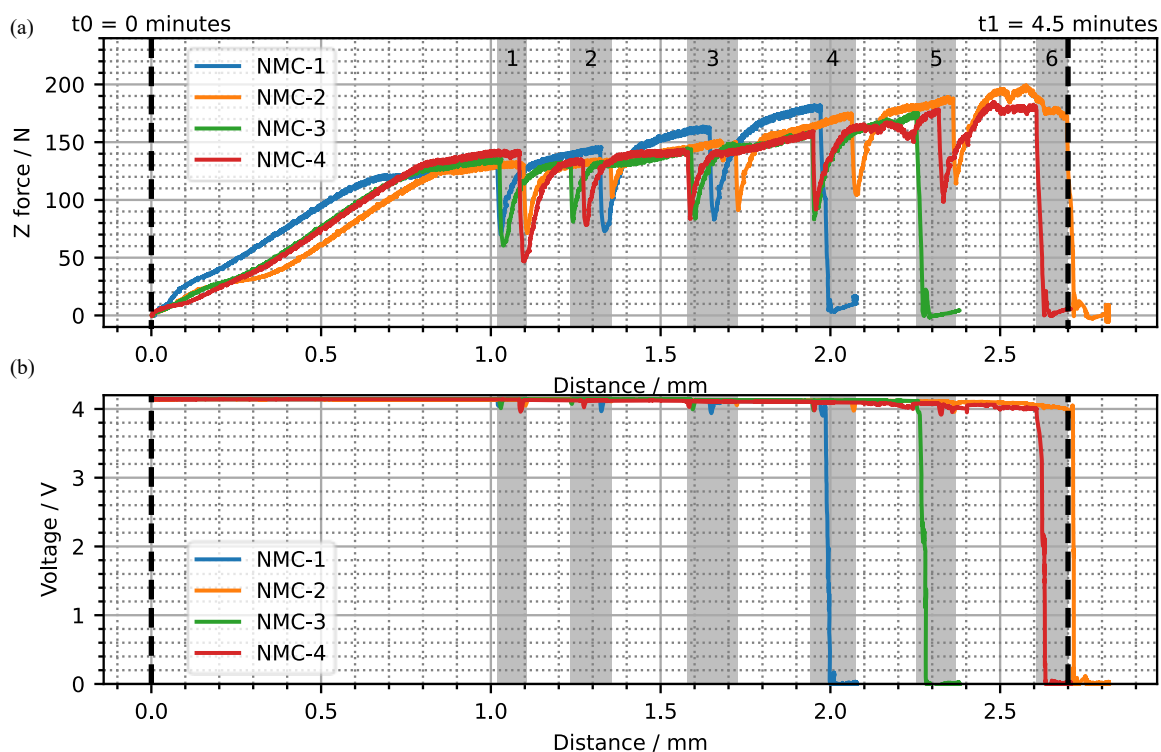


Figure S4: (a) z-Force and from NMC1-4 of NPT at 0.01mm s^{-1} speed with marked short circuits. (b) voltage data from NMC1-4 of NPT at 0.01mm s^{-1} speed with marked short circuits, showing the full voltage range to 0 V.

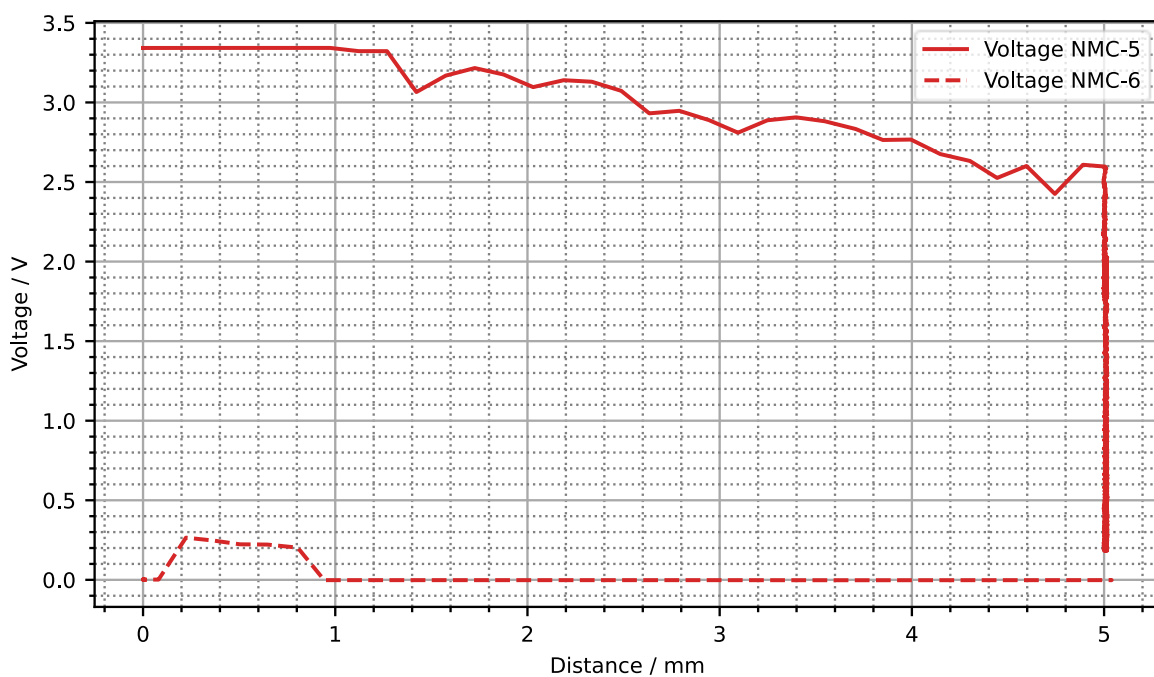


Figure S5: Voltage trend during the NPT of NMC-5 and NMC-6. The NPT of NMC-5 and NMC-6 were conducted at 20°C and after submersion in LN_2 , respectively. Both cells were in a completely discharged state (SOC = 0%). The corresponding force data can be found in Figure 4.

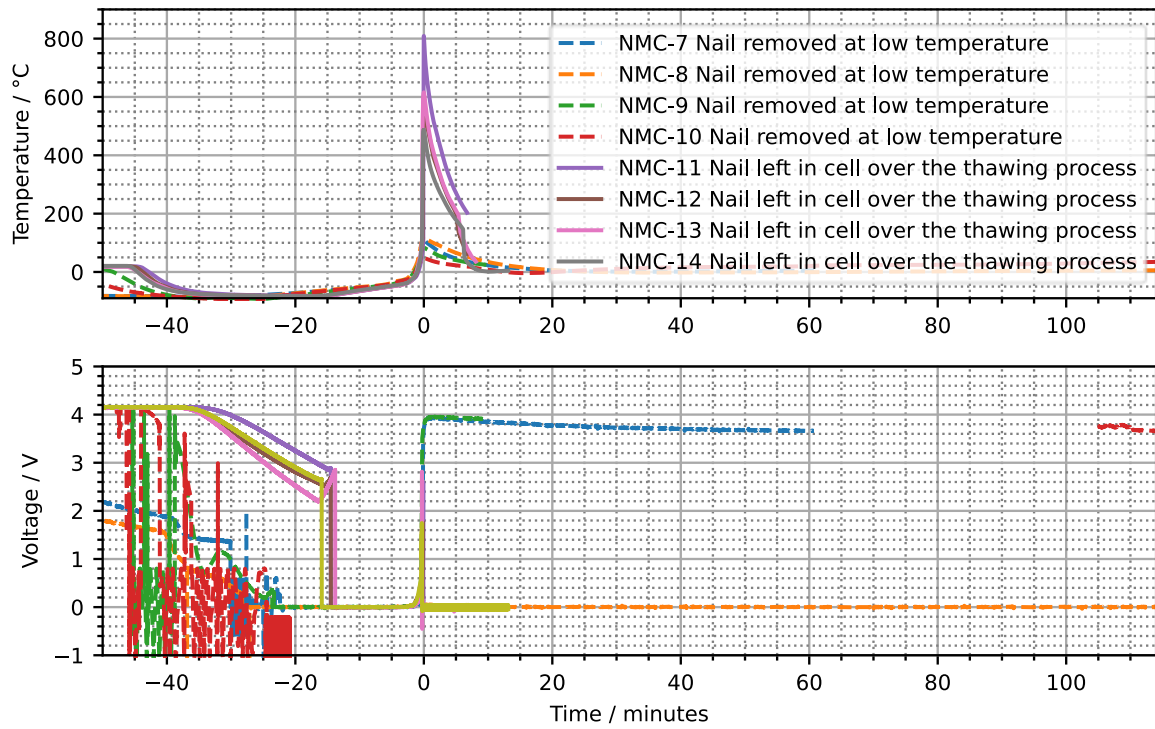


Figure S6: NPT comparison of tests performed at low temperatures with and without nail remaining in cell during rethermalization.

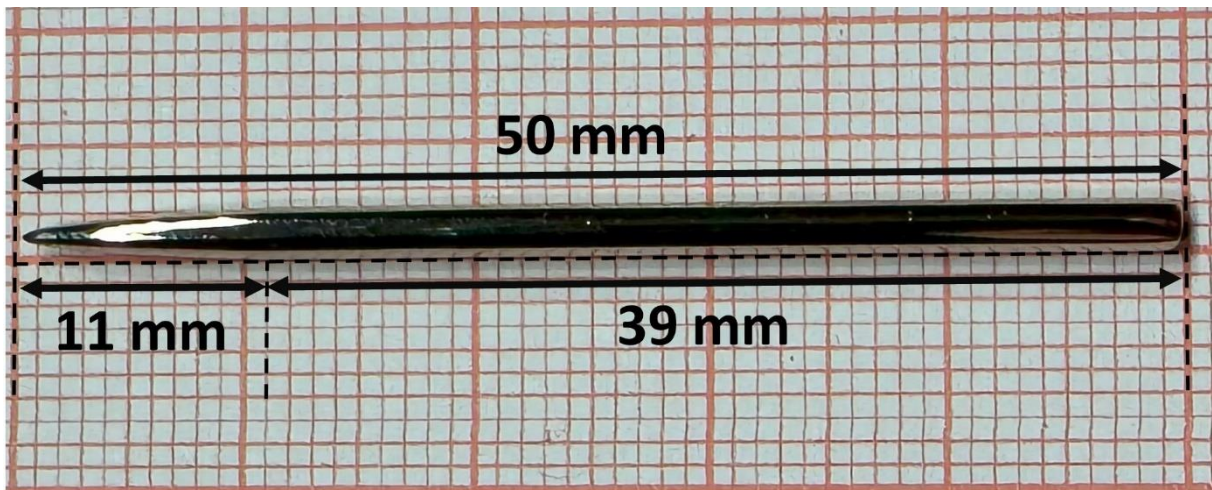


Figure S7: Exemplary photo of one of the dart tips which were used in the present work as nails for all penetration experiments (nail was put on grid paper for the photo; dashed black lines are guides for the eyes). The nail has a total length of 50 mm and a diameter of 2.26 mm. Moreover, the nail has a torpedolike tip with a length of ca. 11mm.