Introduction to ImpedanceFitter

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October 12, 2022

Use case

- Multiple impedance spectra have been recorded
  - Visualization
  - Validity check
  - Fitting, data analysis
- An impedance model is available
  - Expected impedance in a defined frequency range
  - Decomposition of the model
  - Estimating dielectric properties

Advantages

- High-level interface, batch processing
- Flexible choice of fitting algorithm
- Many relevant models implemented

Getting started

- Prerequisite: Python >= 3.6 installed, download from `https://www.python.org`. **Make sure that Python is added to the PATH variable on Windows!**
- Ideally: Jupyter installed (to have Jupyter notebooks) from `https://jupyter.org/`
- Installation is a one-liner:

  pip install impedancefitter
- Bugs? Please report them to me!
- Documentation on the website: `https://impedancefitter.readthedocs.io`
- Feedback is highly appreciated!

General idea

- The impedance measured in electrochemical impedance spectroscopy (EIS) is assumed to be the linear response of the system

$\Rightarrow$ Only linear models (equivalent circuits) considered

- The impedance is modelled by a series or parallel connection of circuit elements and pre-defined circuits
- Realisation in ImpedanceFitter: model is defined in a string and parsed
- Example: Randles circuit

```
model = 'R_s + parallel(R_ct + W, C)'
model = 'Randles'
```

The model

- The model is connects elements in series by + and in parallel by `parallel(a, b)`
- Example: Randles circuit

```
model = 'R_s + parallel(R_ct + W, C)'
model = 'Randles'
```

- Question: find out more about the implementation of the Randles circuit and its parameters on the website
- To compute the impedance: generate an equivalent circuit and evaluate it

```
Z = lmfit_model.eval(omega=2. * numpy.pi *
    frequencies, ct_R=Rct, s_R=Rs, C=C0, Aw=Aw)
```

! If you are new to Python please don't hesitate to ask questions!

Post-processing the model data

- Various functions to plot the data are available: 'plot_admittance', 'plot_bode', 'plot_cole_cole', 'plot_comparison_dielectric_properties', 'plot_complex_permittivity', 'plot_dielectric_dispersion', 'plot_dielectric_modulus', 'plot_dielectric_properties', 'plot_impedance', 'plot_resistance_capacitance'

⇒ Documentation on website or through docstrings

- Every device has a frequency independent unit capacitance C_0, which relates the impedance to the dielectric properties

$$Z = \frac{1}{j\omega\hat{\varepsilon}C_0} \text{ with } \hat{\varepsilon} = \varepsilon_r - \frac{j\sigma}{\omega\varepsilon_0} \quad . \tag{1}$$

⇒ Function: `impedancefitter.utils.return_diel_properties`

EIS data analysis: loading the data

- Available file formats: https://impedancefitter.readthedocs.io/en/latest/examples/fileformats.html

! Reach out to me if you want other file formats to be implemented

- General idea: fixed frequencies in one file, probably multiple impedance spectra (real and imaginary part)
- Other representations (polar, R-C, etc.) need to be converted before loaded
- Simplest starting point:

```
fitter = impedancefitter.Fitter('CSV')
fitter.visualize_data()
fitter.visualize_data(allinone=True)
```

EIS data analysis: validating the data

- Impedance data have to fulfil Kramers-Kronig relations
- Test based on general equivalent circuit[1]
- Automated algorithm is implemented[2]
- Simple interface:

```
results, mus, residuals = fitter.linkk_test()
```

- Test: let's check two exemplary files

[1] Boukamp, B. A. (1995). A Linear Kronig-Kramers Transform Test for Immittance Data Validation. Journal of The Electrochemical Society, 142(6), 1885–1894.

[2] Schönleber, M., Klotz, D., & Ivers-Tiffée, E. (2014). A Method for Improving the Robustness of linear Kramers-Kronig Validity Tests. Electrochimica Acta, 131, 20–27.

EIS data analysis: fitting the data

1. Choose a model
2. Run the fit
3. If real or imaginary part are close to zero, it is better to check the residual with respect to the absolute value of the impedance
4. If the impedance varies a lot with frequency, it is advised to use a weighting algorithm
5. The fit result should be scrutinised by checking the errors of the variables and their correlations in the fit report

EIS data analysis: post-processing the data

- The fit result can be used to compute the impedance of the model and sub-models
- The different impedance of the model and sub-models can be visually compared
- The data can be exported straightforwardly
- If much data has been fitted: ImpedanceFitter can be used to generate histograms (not shown here, please be referred to online documentation)

Applications

Zimmermann, J., et al. (2021) Using a Digital Twin of an Electrical Stimulation Device to Monitor and Control the Electrical Stimulation of Cells in vitro. Front. Bioeng. Biotechnol. 9:765516.

- EIS of a stimulation device
- Extraction of different parameters related to electrical, thermal and (electro-)chemical effects by fitting
- Computation of impedances as input for models

Zimmermann, J., & van Rienen, U. (2021). Ambiguity in the interpretation of the low-frequency dielectric properties of biological tissues. Bioelectrochemistry, 140, 107773.

- Comparison of measured data and a parametric model
- Data analysis and model analysis
- Suggested correction (see `Correction-Ambiguity.ipynb`)