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pyQCM-BraTaDio: A tool for visualization, data mining, and modelling of Quartz crystal microbalance with dissipation data

Brandon Pardi [1], **Syeda Tajin Ahmed** [1], **Silvia Jonguitud Flores** [3], **Warren Flores** [1], **Jean-Michel Friedt** [5], **Laura L. E. Mears** [2], **Bernardo Yáñez Soto** [3], and **Roberto C. Andresen Eguiluz** [1,4¶]

1 Department of Materials Science and Engineering, University of California Merced, Merced, California 95344, United States of America **2** Institute of Applied Physics, Technische Universitaet Wien, Vienna 1030, Austria **3** Instituto de Física, Universidad Autónoma de San Luis Potosí, San Luis Potosí 78000, Mexico **4** Health Sciences Research Institute, University of California Merced, Merced, California 95344, United States of America **5** FEMTO-ST Time & Frequency department, 26 Rue de l'Épitaphe, 25000 Besançon, France ¶ Corresponding author

DOI: 10.21105/joss.06831

Software

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Editor: Bonan Zhu

Reviewers:

- @kstenio
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Submitted: 05 February 2024
Published: 17 July 2024

Summary

Here, we present a Python-based software that allows for the rapid visualization, data mining, and basic model applications of quartz crystal microbalance with dissipation data. Our implementation begins with a Tkinter GUI to prompt the user for all required information, such as file name/location, selection of baseline time, and overtones for visualization (with customization capabilities). These inputs are then fed to a workflow that will use the baseline time to scrub and temporally shift data using the Pandas (McKinney & others, 2010) and NumPy (Harris et al., 2020) libraries and carry out the plot options for visualization. The last stage consists of an interactive plot, that presents the data and allows the user to select ranges in MatPlotLib-generated panels (Hunter, 2007), followed by application of data models, including Sauerbrey, thin films in liquid, among others, that are carried out with NumPy and SciPy (Virtanen et al., 2020). The implementation of this software allows for simple and expedited data visualization and analysis, in lieu of time consuming and labor-intensive spreadsheet analysis.

Statement of need

QCM-D has gained popularity in many different scientific fields due to its experimental simplicity and versatility. QCM-D (or just QCM if not quantifying energy losses) can be combined with a variety of instruments for in situ complementary measurements, such as atomic force microscopy (AFM), (Friedt et al., 2003) microtribometry, (Borovsky et al., 2019) surface plasmon resonance (SPR), (Bailey et al., 2002) or electrochemistry, (Levi et al., 2016) among others. However, one drawback rests in that any QCM-D experiment, real-time monitoring of sensor surface-environment generates large volumes of data entries, and packages used to collect data do not typically possess straightforward data visualization, data mining capabilities, and basic model applications. Furthermore, programs associated with QCM-D data collection and analysis are often proprietary with limited access. There exists other open-source packages, such as RheoQCM (Shull et al., 2020) and pyQTM (Johannsmann et al., 2023), however, they focus on more complex data modeling rather than data mining. `pyQCM-BraTaDio` can serve as a complement to these two packages. Here, we present an intuitive Python-based, open-source software that is QCM-D manufacturer agnostic of multi-harmonic collecting systems for (1)

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simple and fast data visualization and interaction, (2) data mining and reduction, and (3) basic model applications. The supported models include (i) Sauerbrey, for rigid thin films, (ii) viscoelastic thin film in a Newtonian liquid, (iii) viscoelastic thin film in air, and (iv) quartz crystal thickness determination.

Software interaction

Figure 1: User interface of pyQCM-BraTaDio. (1) Initialization conditions, (2) selection of frequencies and dissipation for data mining, visualization, and modeling, (3) interactive plotting options for data range selection, and (4) selection of plotting options and modeling.

The interaction with `pyQCM-BraTaDio` is via a GUI, which allows the user to utilize the software with minimal to no console interaction. It operates following the workflow shown in SI figure 2, The main window is organized into four main regions, shown in Figure 1. These regions are (1) initialization conditions, (2) selection of frequencies and dissipation for data mining, visualization, and model application purposes, (3) interactive plots for data mining, and (4) selection of plotting options and models.

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Notable features of `pyQCM-BraTaDio`

Expedited basic visualizations

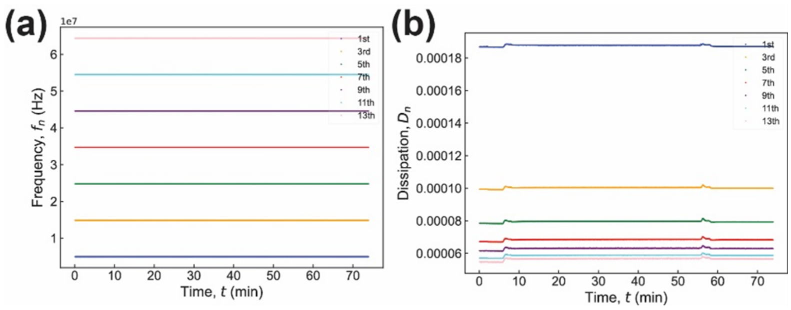

Figure 2: Raw data plots generated by BraTaDio for film formed from a solution of BSA at 1 mg/mL in PBS adsorbed to an Au-coated quartz crystal. (a) Absolute frequency f_n as a function of time t, (b) corresponding absolute dissipation D_n as a function of time for $n =$ 3, 5, 7, 9, 11, and 13. The peaks seen in panel (b) correspond to transition periods, that is, pumping BSA after the PBS baseline was established ($t =$ 5 min), and the second to a PBS wash ($t =$ 55 min).

As in any experimentally obtained data, visual inspection is crucial for an initial assessment of baseline stability, anomalies, such as presence of undesired air bubbles, leaks, signal loss, among others. Two basic visualization options are implemented in the `pyQCM-BraTaDio` tool: (i) a full data range visualization referred here as raw data, Figure 2, and (ii) the experimental data, referred here as reference level adjusted data, Figure 3. For these options, the user can select the overtone order(s) to visualize the frequency and dissipation in various plotting formats. Figure 2(a) and (b) show the absolute frequency f_n and dissipation D_n as a function of time t for $n = 1, 3, 5, 7, 9, 11$ and 13 for a bovine serum albumin (BSA) solution absorbing to a gold substrate. The relevant experimental data can be visualized by selecting the 'Plot shifted data' option. For example, change in frequency as a function of time, Δf_n vs time t, Figure 3(a), change in normalized frequency as a function of time, $\Delta f_n/n$ vs time t, Figure 3(b), change in dissipation ΔD_n vs time t, Figure 3(c), combined change in frequency and change in dissipation as a function of time, Δf_n and ΔD_n vs time t, Figure 3(d), combined change in normalized frequency and change in dissipation as a function of time, $\Delta f_n/n$ and ΔD_n vs time t, Figure 3(e), the temperature T as a function of time, T vs t, Figure 3(f), which is critical to determine any temperature effects in collected data. Finally, change in dissipation as a function of change in frequency, ΔD_n vs Δf_n, Figure 3(g), and change in dissipation as a function of change in normalized frequency, ΔD_n vs $\Delta f_n/n$, Figure 3(h) to obtain qualitative insights of the adsorbed film rigidity.

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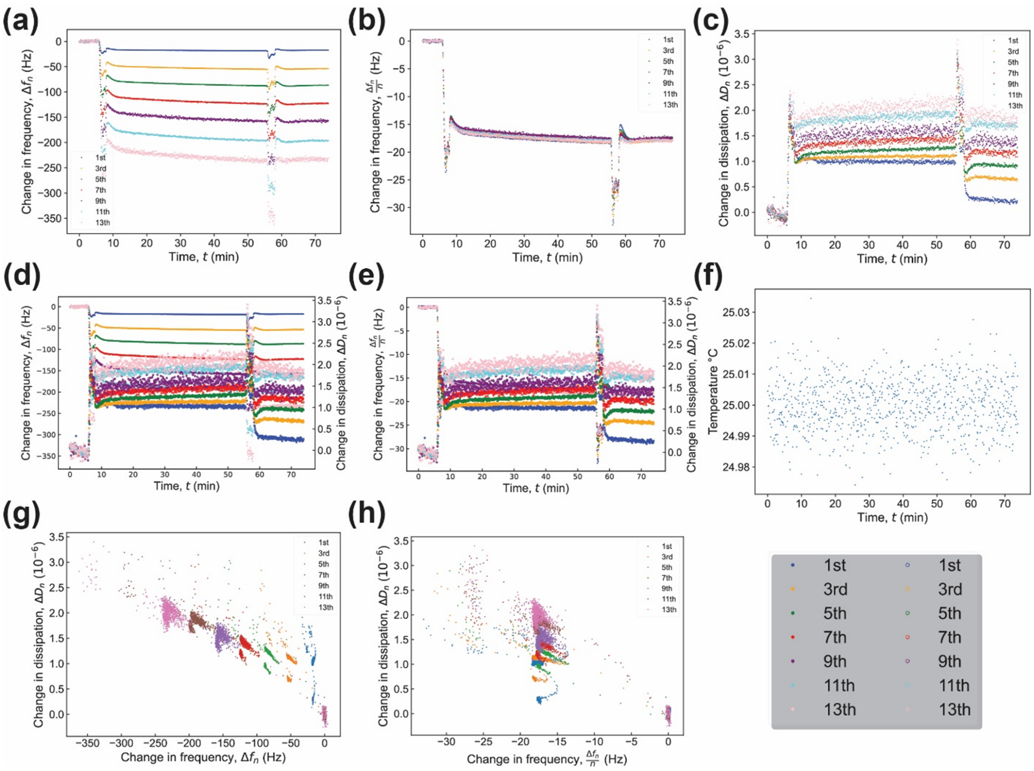

Figure 3: Plots generated by BraTaDio for a film formed from a solution of BSA at 1 mg/mL in PBS adsorbed to an Au-coated quartz crystal. (a) Change in frequency Δf_n as a function of time t, (b) change in frequency normalized by overtone order, $\Delta f_n/n$ as a function of time t, (c) corresponding change in dissipation ΔD_n as a function of time, (d) change in frequency Δf_n and corresponding change in dissipation ΔD_n as a function of time, (e) change in frequency $\Delta f_n/n$ normalized by overtone order and corresponding change in dissipation ΔD_n as a function of time, (f) temperature T as a function of time, (g) change in dissipation ΔD_n as a function of change in frequency, $\Delta f_n/n$ and (h) change in dissipation ΔD_n as a function of change in frequency normalized by overtone order, $\Delta f_n/n$. Data collected with a QCM-I system.

Data mining via an interactive plot (Figure 4)

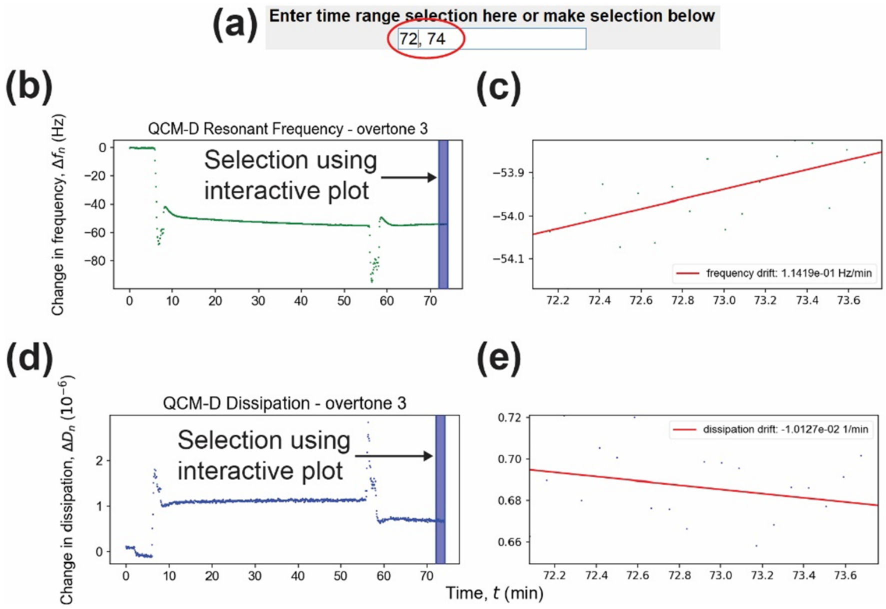

Figure 4: The interactive plot of pyQCM-BraTaDio. (a) Input line for time range selection, (b) change in frequency interactive plot, (c) zoomed-in region from the change in frequency interactive plot and frequency drift, (d) change in dissipation interactive plot, and (e) zoomed-in region from the change in dissipation interactive plot and dissipation drift.

To facilitate the procedure of data mining (Figure 4), that is, selection of frequency and dissipation ranges for time ranges of interest, it is possible to interact with the data via an interactive plot. pyQCM-BraTaDio will compute the average and standard deviation of the data points contained within the selected range for each overtone selected and display the selection with a linear fit, every time a selection is made. Through the use of user dictated range identifiers, multiple selections can be made without overwriting data. Overwriting only occurs when further selections are made without updating the range identifier *ex ante* (Figure 4)

Applications of models

Matching QCM-D experimental data to models that provide physical interpretation is key for the quantitative characterization of liquids interacting with the quartz crystal surfaces or nanofilms. With `pyQCM-BraTaDio`, it is possible to apply models of steady state (in equilibrium) thin films using one of the following models: (i) the Sauerbrey equation for very thin films, (Sauerbrey, 1959) (ii) shear-dependent compliance of a thin viscoelastic film in a Newtonian liquid, (Du & Johannsmann, 2004) and (iii) determination of the quartz crystal thickness. (Reviakine et al., 2004) These models are described in the SI, accompanied with experimental examples.

Conclusions

pyQCM-BraTaDio is a Python software implemented ad hoc to expedite the process of data mining and analysis of QCM-D experimental data. Beginning with a Tkinter GUI for metadata collection, the inputs and data are fed to several routines to mine and reference level adjust data with the Pandas and NumPy libraries. The user is able to interact with QCM-D data in a novel way via a Matplotlib interactive plot widget towards the end of the workflow. This interaction offers the user to apply several models such as Sauerbrey, thin film in liquid, thin film in air, and crystal thickness. This tool is key for efficient data analysis in preference over laborious spreadsheet evaluation.

Author contributions

Conceptualization: Brandon Pardi, Syeda Tajin Ahmed, Roberto C. Andresen Eguiluz; data curation: Syeda Tajin Ahmed, Silvia Jonguitud Flores, Warren Flores, Bernardo Yáñez Soto, Roberto C. Andresen Eguiluz; formal analysis: Brandon Pardi, Syeda Tajin Ahmed, Jean-Michel Friedt, Laura L.E. Mears, Bernardo Yáñez Soto, Roberto C. Andresen Eguiluz; funding acquisition: Bernardo Yáñez Soto, Roberto C. Andresen Eguiluz; investigation: Brandon Pardi, Syeda Tajin Ahmed, Roberto C. Andresen Eguiluz; methodology: Brandon Pardi, Syeda Tajin Ahmed, Jean-Michel Friedt, Bernardo Yáñez Soto, Roberto C. Andresen Eguiluz; project administration: Brandon Pardi, Roberto C. Andresen Eguiluz; resources: Brandon Pardi, Syeda Tajin Ahmed, Laura L.E. Mears, Bernardo Yáñez Soto, Roberto C. Andresen Eguiluz; software: Brandon Pardi, Jean-Michel Friedt; supervision: Brandon Pardi, Bernardo Yáñez Soto, Roberto C. Andresen Eguiluz; validation: Brandon Pardi, Syeda Tajin Ahmed, Silvia Jonguitud Flores, Warren Flores, Jean-Michel Friedt, Laura L.E. Mears, Bernardo Yáñez Soto, Roberto C. Andresen Eguiluz; visualization: Brandon Pardi, Syeda Tajin Ahmed, Laura L.E. Mears, Roberto C. Andresen Eguiluz; writing & original draft: Brandon Pardi, Syeda Tajin Ahmed, Silvia Jonguitud Flores, Bernardo Yáñez Soto, Roberto C. Andresen Eguiluz; writing & review & editing: Brandon Pardi, Syeda Tajin Ahmed, Silvia Jonguitud Flores, Laura L.E. Mears, Bernardo Yáñez Soto, Roberto C. Andresen Eguiluz.

Conflicts of interest

The authors declare no conflicts of interest.

Acknowledgements

R.C.A.E. acknowledges funding from the NSF-CREST: Center for Cellular and Biomolecular Machines through the support of the National Science Foundation (NSF) Grant No. NSF-HRD-1547848. R.C.A.E. and B.P. acknowledge funding from the CAREER grant NSF CMMI Grant No. #2239665 awarded to R.C.A.E. R.C.A.E. and W.F. acknowledge funding from the LEAP HI grant NSF CMMI Grant No. #2245367 awarded to R.C.A.E

Supporting information

The authors have compiled additional supporting information in a separate document containing more details on the software's execution, as well as demonstrating the efficacy of the software across multiple QCM-D devices.

References

Bailey, L. E., Kambhampati, D., Kanazawa, K. K., Knoll, W., & Frank, C. W. (2002). Using surface plasmon resonance and the quartz crystal microbalance to monitor in situ the interfacial behavior of thin organic films. *Langmuir*, *18*(2), 479–489. https://doi.org/10.1021/la0112716

Borovsky, B., Garabedian, N., McAndrews, G., Wieser, R., & Burris, D. (2019). Integrated QCM-microtribometry: Friction of single-crystal MoS2 and gold from μm/s to m/s. *ACS*

Applied Materials & Interfaces, *11*(43), 40961–40969. https://doi.org/10.1021/acsami.9b15764

Du, B., & Johannsmann, D. (2004). Operation of the quartz crystal microbalance in liquids: Derivation of the elastic compliance of a film from the ratio of bandwidth shift and frequency shift. *Langmuir*, *20*(7), 2809–2812. https://doi.org/10.1021/la035965l

Friedt, J.-M., Choi, K.-H., Frederix, F., & Campitelli, A. (2003). Simultaneous AFM and QCM measurements: Methodology validation using electrodeposition. *Journal of The Electrochemical Society*, *150*(10), H229. https://doi.org/10.1149/1.1603255

Harris, C. R., Millman, K. J., Van Der Walt, S. J., Gommers, R., Virtanen, P., Cournapeau, D., Wieser, E., Taylor, J., Berg, S., Smith, N. J., & others. (2020). Array programming with NumPy. *Nature*, *585*(7825), 357–362. https://doi.org/10.1038/s41586-020-2649-2

Hunter, J. D. (2007). Matplotlib: A 2D graphics environment. *Computing in Science & Engineering*, *9*(3), 90–95. https://doi.org/10.1109/mcse.2007.55

Johannsmann, D., Langhoff, A., Leppin, C., Reviakine, I., & Maan, A. M. (2023). Effect of noise on determining ultrathin-film parameters from QCM-d data with the viscoelastic model. *Sensors*, *23*(3), 1348. https://doi.org/10.3390/s23031348

Levi, M. D., Daikhin, L., Aurbach, D., & Presser, V. (2016). Quartz crystal microbalance with dissipation monitoring (EQCM-d) for in-situ studies of electrodes for supercapacitors and batteries: A mini-review. *Electrochemistry Communications*, *67*, 16–21. https://doi.org/10.1016/j.elecom.2016.03.006

McKinney, W., & others. (2010). Data structures for statistical computing in python. *Proceedings of the 9th Python in Science Conference*, *445*, 51–56. https://doi.org/10.25080/majora-92bf1922-00a

Reviakine, I., Morozov, A. N., & Rossetti, F. F. (2004). Effects of finite crystal size in the quartz crystal microbalance with dissipation measurement system: Implications for data analysis. *Journal of Applied Physics*, *95*(12), 7712–7716. https://doi.org/10.1063/1.1737049

Sauerbrey, G. (1959). Verwendung von Schwingquarzen zur Wägung dünner Schichten und zur Mikrowägung. *Zeitschrift Fur Physik*, *155*(2), 206–222. https://doi.org/10.1007/BF01337937

Shull, K. R., Taghon, M., & Wang, Q. (2020). Investigations of the high-frequency dynamic properties of polymeric systems with quartz crystal resonators. *Biointerphases*, *15*(2). https://doi.org/10.1116/1.5142762

Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., … SciPy 1.0 Contributors. (2020). SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python. *Nature Methods*, *17*, 261–272. https://doi.org/10.1038/s41592-019-0686-2