# Documentation

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# Introduction

## GUI Overview

This **Graphical User Interface** is designed for Determining the **Crystallization Dynamics** and **Kinetics** of substances using a simple **S11** parameter obtained from **NanoVNA** (Affordable and Portable) Interfaced to crystal holder containing the Quartz Crystal. **S11** is the parameter used to determine the how much signal reflected back to device, **S21** is used to transmit the signal to test the process of signalling is working or not and filtering the peak to detect the sharper peaks.

There are many Software's in the internet including the **NanoVNA-Saver** by **NanoVNA** (Constantly and Consistently Upgraded by the contributors in the World as it is an open-source software), they gather the data or parameters from the device through **batches**, but none of them do dynamics or kinetics for the Solutions.

This GUI fills those empty holes, by **determining crystallization dynamics (Rate at which Crystal's form and grow) and kinetics (Description of Rate laws governing nucleation) using the correlated Models** such as **BVD (Butterworth Van-Dyke Model), Avrami Model, Phase Shift method, Sauerbrey and Kanazawa Equations**. From these models, Significant Graphs that are correlated with the process are also plotted to determine the Growth Rates, Nucleation Onset.

## Extraction and Parsing the Parameter

The two parameters S11 and S21 can be acquired from NanoVNA using the commands such as data0, data1 respectively. Acquiring these values depends on how many ports our system is connected to. If it is connected to one port, through system or command, we can acquire only one value (S11 Reflection coefficient). If it is connected to two ports, then we can acquire S11 and S21. However, S21 is preferred for measurements in BVD and all Other analysis tools as it will show clear peak or dip in the graphs. The values from these data commands will be real and imaginary parts, using these values, we can evaluate impedance, which is the main parameter to be used in the future work. Evaluation of impedance from S21 depends on how our system is coupled in series or parallel(shunt) with transmission line.

**Series Setup:** The components connected end to end, forming a single path for current flow

**Shunt or Parallel Setup:** The components connected side by side, providing multiple paths for current.

Mostly systems or setup used will be series setup. The formula below mentioned will be used to find impedance from S21 for a series setup.

$$Z = 2Z_0 \frac{(1-S21)}{S21} \qquad \text{………… (1)}$$

If it's a one port connection,

$$\boxed{Z_f = \left(\frac{1+S11}{1-S11}\right) * Z_0}$$

This is the formula we use to find impedance from S11. To determine whether the setup is series or parallel is by watching the screen of data on NanoVNA, for a series setup, S21 has peak, S11 has a dip. For parallel, it is vice-versa.

# Methods

This section pushes more information about the models and the plots, how they are correlated with electrical parameters.

## Butter-van Dyke Model

### Overview

This model is used for determining the dynamics of crystallization by using the **electrical parameters**. These electrical parameters are determined from S21 parameter acquired from the NanoVNA device. **S21 parameter gives the impedance as a complex number**. This complex number contains resistance as real part and reactance as the imaginary part

$$\boxed{Z = R + j X} \qquad \text{………. (2)}$$

The Resistance extracted from the Impedance and the frequency range or an array of values from the device were used to determine the electrical parameters using **BVD (Butterworth**

$$Z_p = -j\frac{1}{2\pi f C_p}$$

**Van-Dyke Model)**

This model has two arms of circuits in parallel with one another (**Static arm and Motional Arm**). The static arm which contains **shunt capacitance Cp,** cannot be used to determine the dynamics, it is used just for determining capacitance across the device. So, we consider motional arm of model for dynamics. This motional arm manages the **motional parameters (Inductance ($L_m$), Capacitance ($C_m$), Resistance ($R_m$)).**

$$\boxed{Z_s = R_m + j(2\pi f L_m - \frac{1}{2\pi f C_m})} \quad \text{.............. (3)}$$

## Fitting and Calculation

Firstly, we need to determine the impedance for every S21 parameter value from the NanoVNA device. This can be achieved by using the eqn (1).

After measuring the impedance, as it is a complex number after the calculation, we need to extract the real part of the impedance which is referred to as **motional resistance ($R_m$).** ***Resonant frequency(f)*** is the minimum value of impedance. Next step is to find the ***Quality Factor (Q). Change in frequency ($\Delta f$)*** is determined through half power method

## Half-Power

**Half-Power is the half of maximum power** i.e. $\boldsymbol{P = \frac{P_{max}}{2}}$. **Half-power points** are defined as frequencies where power delivered is half of power at resonance ***(In other terms $f_1, f_2$ are the frequencies where system is half as efficient (half as power))***. where $\boldsymbol{P \propto \frac{1}{R}}$ ***(This applies when Voltage is constant).***

However, this method not always going to work, because Impedance is not the data, we are acquiring from the equipment which could be continuous but it isn't so we consider $\boldsymbol{\sqrt{2}R_m}$. This R is used as cross reference for half power line, we find the most accurate crossing line, which is used later to find ***Change in frequency ($\Delta f$)*** using Interpolation Technique. After having the calculated parameters, we find Q using the below formula. From Q, we find Inductance and Capacitance using the below formulas.

**Note:** $\boldsymbol{R_m}$, $\boldsymbol{C_m}$, $\boldsymbol{L_m}$ is referred to as ***R, C, L***

$$\boxed{\begin{array}{c} Q = f/\Delta f \\ \Delta f = f_1 - f_2 \end{array}} \qquad \boxed{\omega = 2\pi f} \qquad \boxed{\begin{array}{c} L = QR/\omega \\ C = 1/\omega QR \end{array}}$$

Now, we have L, C, R values. These values are substituted into *Equation 3* as the initial guess, refine it using ***least squares method (Comparing the Measured Impedance from NanoVNA and Modelled Impedance using calculated L, C, R values)*** to find the accurate value of impedance and L, C, R values.

### Correlation of Parameters

This section describes how the above calculated parameters determines the dynamics of crystallization. $\boldsymbol{R_m}$ correlates to dissipation of oscillation energy from structures and from medium in contact with crystal. $\boldsymbol{L_m}$ correlates with inertial component of oscillation, which is related to mass displaced during the vibration. $\boldsymbol{C_m}$ correlates with storage of energy and is related to elasticity of quartz.

## Avrami Model

### Overview

This model is used to determine crystallization kinetics from Resonance Frequency

### Fitting and Calculation

Avrami Model determines the growth rate and mechanism. The *Equation 4* talks about the rates and mechanisms with k, n values.

$$\boxed{\boldsymbol{X(t) = e^{-kt^n}}} \qquad \textbf{...... (4)}$$

Using the *Equation 5*, we find Crystallinity using Resonance frequency values evaluated from S11 as described in BVD Model.

$$X(t) = \frac{f_t - f_0}{f_\infty - f_0} \qquad \text{........ (5)}$$

This crystallinity value from (5) is substituted in (4) to find k, n values. Then again in same procedure as in ***BVD***, using ***curve fitting method***, we accurately predict the k, n values.

### Correlation of Parameters

This section describes how the above calculated parameters determines the dynamics of crystallization. Crystallinity w.r.t time shows how the crystallization happens from initial stage (Nucleation), Middle Stage (Growth), Final Stage (Near Completion). n value suggests that Growth mechanism such as Spherical, plate like, needle like growths

## Phase Shift Method

This is one of the methods used to determine electrical parameters by measuring frequencies at ***phase angles of 0 °, -45 °, and +45 °***. This is one of the easiest and Quickest methods to detect electrical parameters. However, the method comparison with BVD, we can't tell exactly which method is more accurate. But with the parameters and more data, the BVD model could be accurate. Coming to this method, we need to determine ***logmag, dB of S21 parameter***, using these values, we determine the phase, frequencies at different phase values. These phase, frequency values were used to determine ***Rm, Cm, and Lm***, using below formulas

$$S21\,dB = 20\log(|S21|)$$

$$|S21| = \sqrt{Real^2 + Imaginary^2}$$

$$\Delta f = |f_{45} - f_{-45}|$$

$$R_{eff} = 2R_0 + R_m$$

$$phase = \frac{180}{\pi}.arctan(Img, Real)$$

$$C_m = \frac{\Delta f}{2\pi f_0^2 R_{eff}}$$

$$L_m = \frac{R_{eff}}{2\pi \Delta f}$$

$$R_m = 2R_0(10^{\frac{-S21(0)}{20}} - 1)$$

## Sauerbrey and Kanazawa Equations

These equations were solely used to determine the mass load, viscosity and Dissipation.

### Sauerbrey Equation

This equation is used to determine the mass change. We will have known values of ***Density of quartz*** $(\rho_q)$ ***, Shear modulus of quartz (***$\mu_q$***), Change in frequency can be found from resonance values, and Active Area of Electrode (A).***

$$\boxed{\Delta f = \frac{2 f_0 \Delta m}{A\sqrt{\rho_q \mu_q}}}$$

$$\boxed{\Delta m = C\Delta f}$$

### Kanazawa Equation

***Using Kanazawa model, we can find viscosity of solution using this equation similarly to Sauer brey equation.***

$$\boxed{\Delta f = {f_0}^{3/2}\sqrt{\frac{\rho\eta}{\pi\mu_q\rho_q}}}$$

$f_0$ is initial resonant frequency when it is in air or without loading. It does change every time the experiment runs, so we need to note the value from the screen of NanoVNA and use it for evaluation when mass loaded.

## Noise Filtering

Smooth spline filter is noise filtering or smoothing the signal (or graphs) for better performance for every model. There are other methods for filtering the noise such as Savitzky, FIR, IIR, Median, Wavelet. Every Method mentioned has their own pros and cons based on the type of curve or signal we get.

## GUI Process

There are commands for every electrical equipment to communicate their data. They can communicate it through ASCII or USB serial port communications. NanoVNA is one of the devices that communicates the information through ASCII. Every device has their own commands of communication like if we send command ***'info'*** it will give the information of the equipment. ***(It can be verified through Putty or Tera port communication terminal).*** These are some of the commands that we can use to communicate with NanoVNA. Mentioned commands are main prompt commands for this GUI communication but there are many more.

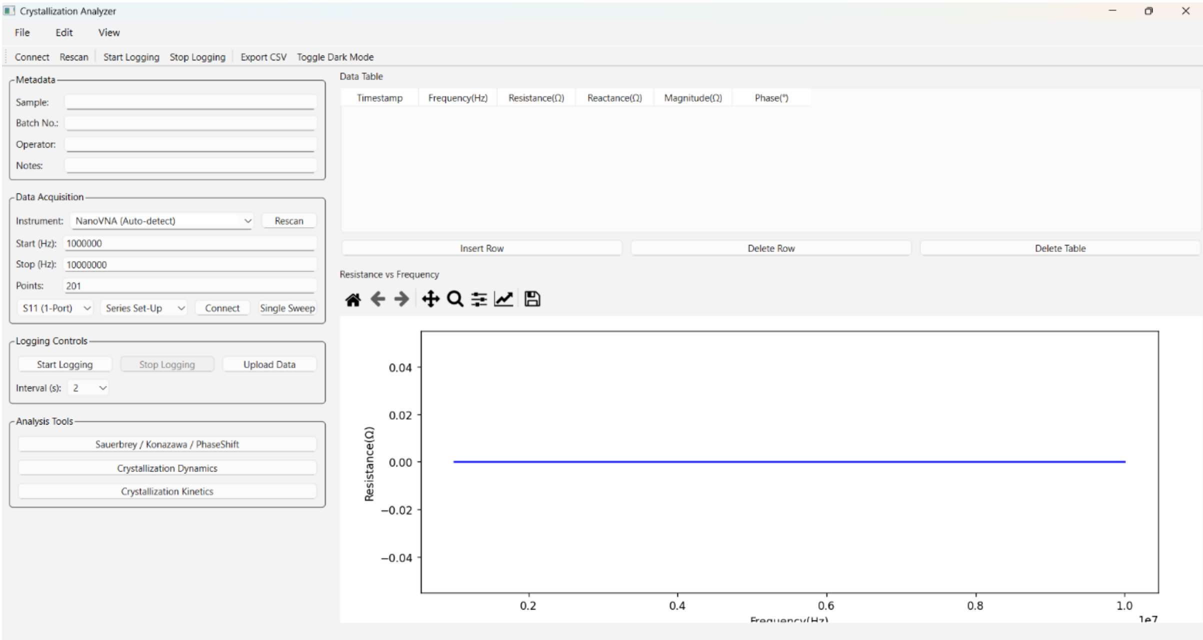
| **Command** | **Communicate** |
|---|---|
| info | Device name and other information |
| sweep | It provides ***start stop sweep points*** |
| data | It gives the data in the format of real and imaginary parts side by side |
| freq | Frequency |
| data 0 | Usually S11 parameter (real and imaginary parts) |
| data 1 | S21 parameter |

Using these commands coded a file with communicating and by pyserial language to code for connecting through the equipment.

After communicating with equipment, the data will be acquired. This data will be refined to give impedance and other key parameters for crystallization dynamics and kinetics analysis as discussed above in the methods. For clear explanation of code execution, you can screen through GitHub repo.

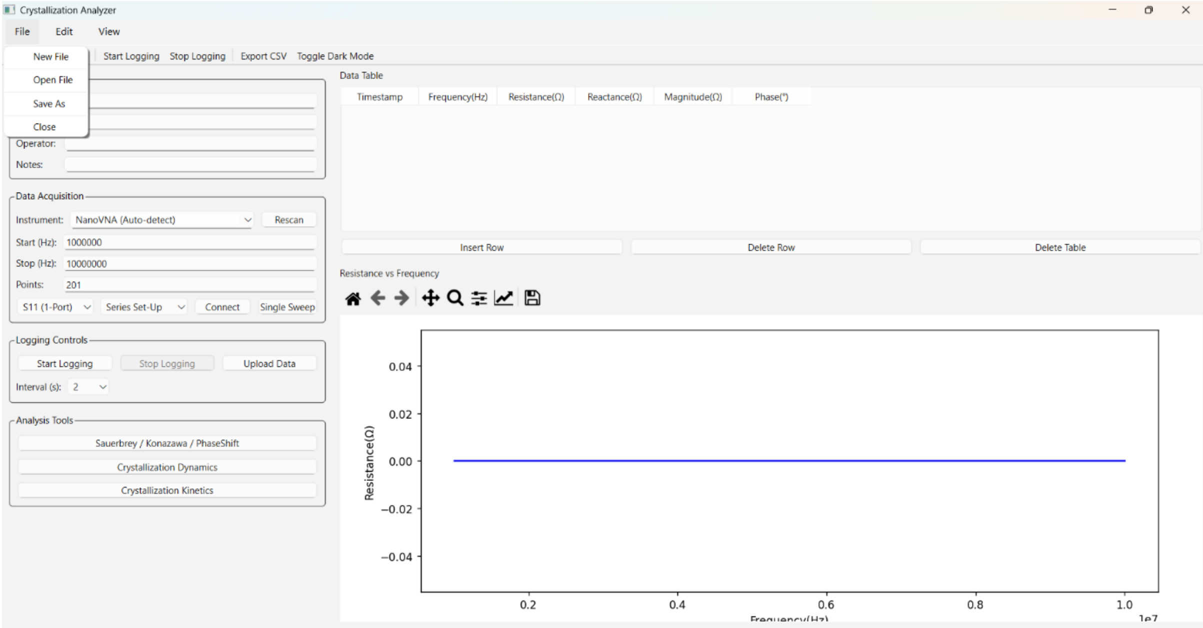
# GUI Work

## Homepage




Above screenshot is a homepage of the GUI, it can be seen with many features such as ***File, Edit, View Menu bar***. An easy access of some buttons for the users in the toolbar with (Connect, Rescan, Start and Stop Logging) *Controls for the NanoVNA*, ***Export CSV*** is for exporting the table content in csv file, ***Dark Mode*** is for visual appearance. It has some other features such as ***Metadata*** (user can save their samples with metadata), ***Data Acquisition*** (Controlling the equipment connection and setting the frequency range), ***Logging Controls*** (User can start and stop logging the data whenever they want and User can also upload their own data without connecting to the equipment, User can also choose the interval of logging the data continuously). ***Analysis tools*** (User can find crystallization dynamics and kinetics of the solution). On the right side, User can see the ***acquired data in a table form*** and a ***graph for Resistance vs Frequency***. After ***connected to NanoVNA***, to run a single sweep or start logging, user need ***to choose port (S11, S21)***, based on the ***connection discussed in Introduction***.

## File Menu




When a user clicks on ***File menu***, he can able to ***create a new file and open an existing file*** in their computer, save the file of whole data in an ***PDF format using Report Lab***. When the user clicks the new file, it will create a new file. If Open is clicked, User needs to ***upload a CSV*** file of ***Resistance, Frequency and Timestamp of data***. So that whole GUI works on this data. If user clicks Save As, it will create a ***ZIP folder containing plots images, PDF, CSV files of Table Data from crystallization Dynamics and Basic Data Table created using S-Parameter***

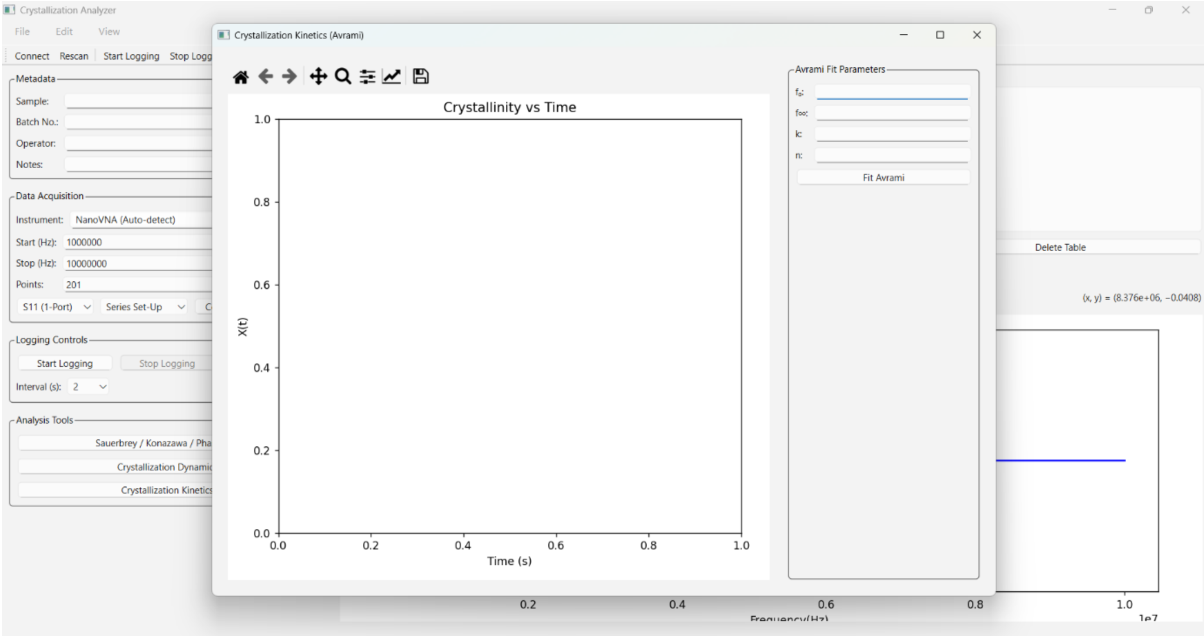
## Edit Menu

In the edit menu, it is a simple visual appearance button which is dark mode

## View Menu

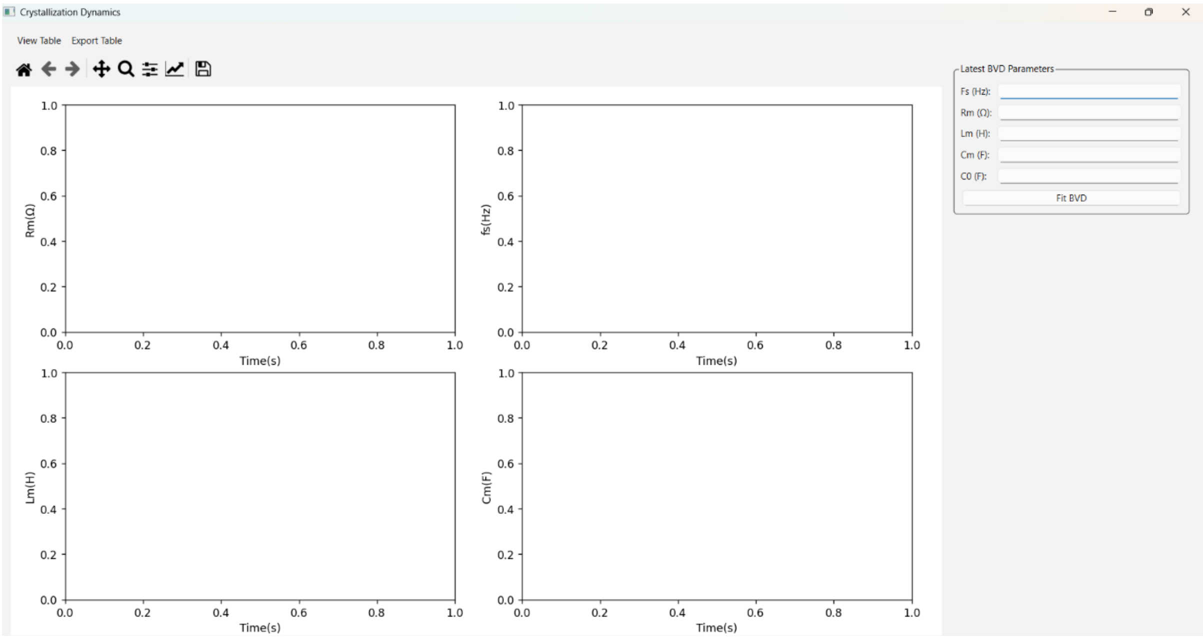
View menu has Add table and export CSV, user can able to add their own table of data and edit the data in the table and also export csv option enables the user to export all the table data from every window into csv files

## Crystallization Kinetics



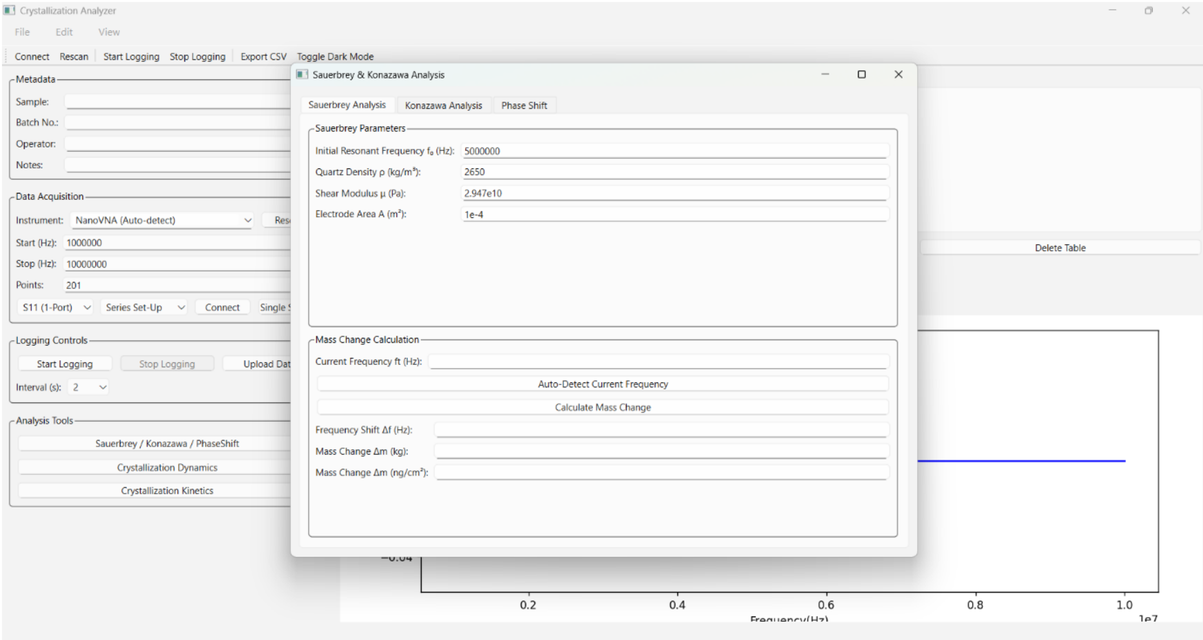

When a user clicks for ***kinetics tool***, going to ***pop a crystallization kinetics window*** with ***Crystallinity vs time*** graph and on the ***right*** side, user can able to edit the ***parameter*** data obtained to fit the Avrami Model.

## Crystallization Dynamics



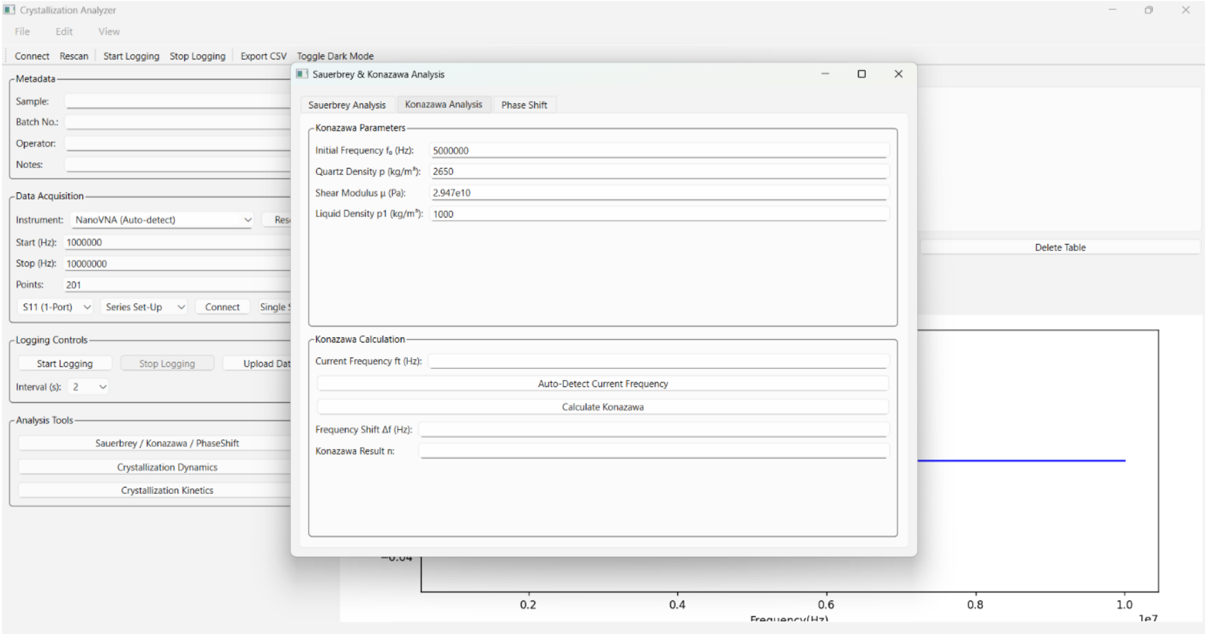

When a user clicks for dynamics, similar to crystallization kinetics, there will be window, which has view Table data obtained for dynamics containing Rm, Lm, Cm, Fs and export table data. On the Left-Hand Side, it has Four Plots, Motional Resistance Vs Time, Motional Inductance vs Time, Motional capacitance vs Time, Resonance Frequency vs Time. And on the right side, Calculated parameters and fitting BVD model.

## Sauerbrey Analysis



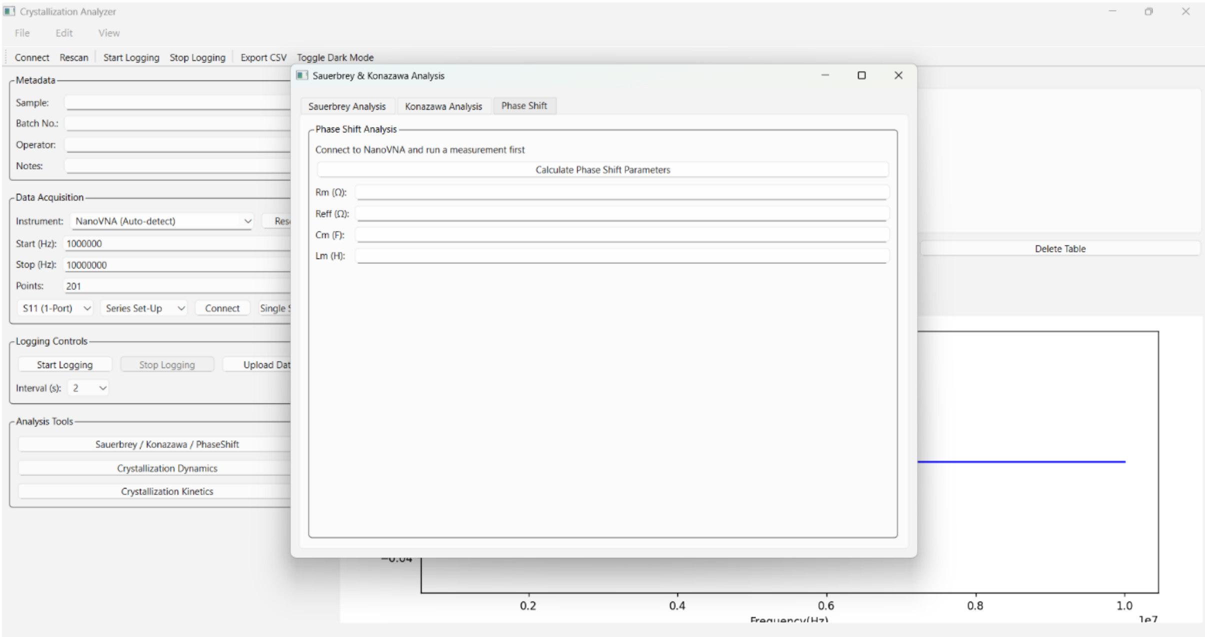

When the user clicks on Sauerbrey/Konazawa/Phase shift Tool, it opens a window containing Sauerbrey, Konazawa, Phase Shift. If the User clicks on Sauerbrey Analysis, It has parameters Resonant Frequency, Quartz Density, Shear Modulus, Electrode Area. These are defined parameters, But User need to be careful of Initial resonant frequency, User need to measure when the mass is not loaded, update the value in initial resonant frequency before calculating mass change and frequency shift.

## Konazawa Analysis




If the user clicks on Konazawa Analysis, it has some similar parameters like Sauerbrey. Again, User needs to update the Initial Resonance Frequency as discussed in Sauerbrey analysis section. Using the parameters user can able to calculate viscosity.

## Phase shift




If the user clicks on the Phase shift, it calculates S21 logmag, phase internally and can be used to calculate Rm, Lm, Cm and can be verified with Butterworth Van dyke Model.

# References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