

# The Equivalent Circuit Model and Methods for Finding the Initial Guesses

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September 27, 2022

## 1 The Equivalent Circuit of the Perovskite Device

The equivalent circuit of the perovskite is shown in the plot below. The reasoning behind the equivalent circuit is explained in the paper[ref].

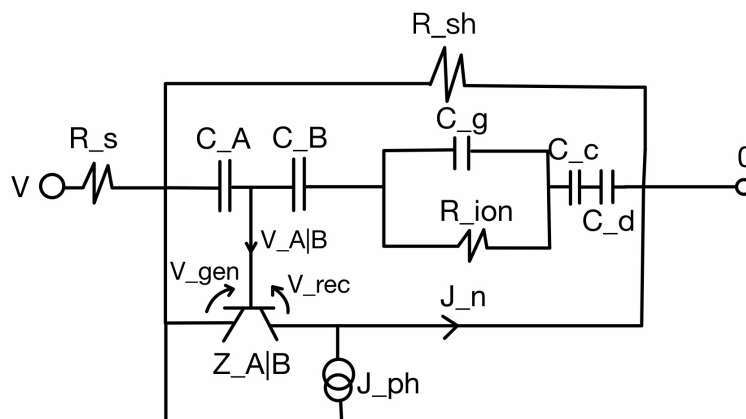


Figure 1: The equivalent circuit of the perovskite device. The meanings of the parameters are listed in the later parts.

By using this circuit, the corresponding function takes in the frequency of the perturbation voltage as the independent variable and returns the impedance

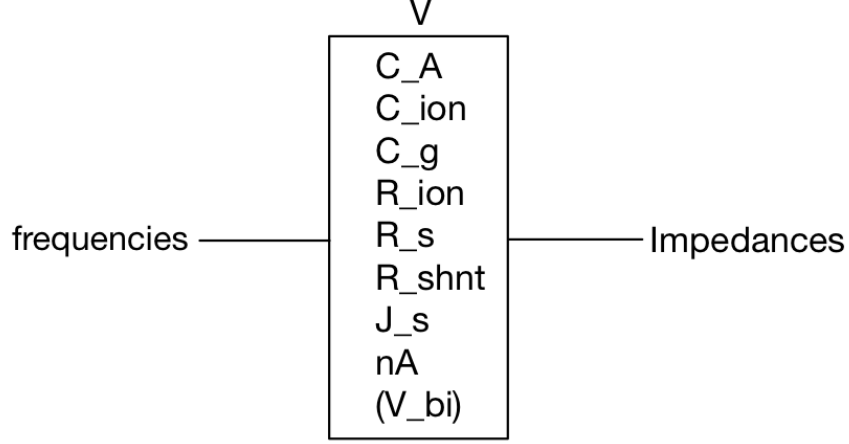


Figure 2: This is the schematic plot of the model. With the given parameters, the model will take in a list of frequencies and output a list of impedances.

of the whole circuit, with given parameters  $C_A$ ,  $C_{ion}$ ,  $C_g$ ,  $R_{ion}$ ,  $R_s$ ,  $R_{sh}$ ,  $J_s$ ,  $nA$  and  $V_{bi}$  (for global fit cases) as shown in Fig. 2.

$C_A$ ,  $C_g$ ,  $R_{ion}$ ,  $R_s$ , and  $R_{sh}$  are elements shown in the circuit, while  $C_{ion}$  is the capacitance of the ionic branch(not including  $C_g$ ),  $J_s$  is the saturation current density, and  $nA$  is the ideality factor of the transistor. The calculation of the total impedance includes using basic electronics laws and the property of the transistor. The detailed derivation is shown in the paper[refff].

## 2 The Initial Guess Finding Function

### 2.1 Individual Fit for Non-0 Bias Voltage

A set of initial guesses can be obtained from the data directly by extracting some important information using different plot representations.

In order to find the initial guess, the important points in the plots are extracted, including  $R_{n\infty}$ ,  $R_{n0}$ ,  $\omega_n$  and  $C_G$ . By using these points, relations illustrated in the paper[refff], and a guess of  $R_{ion}$  by the user, the initial

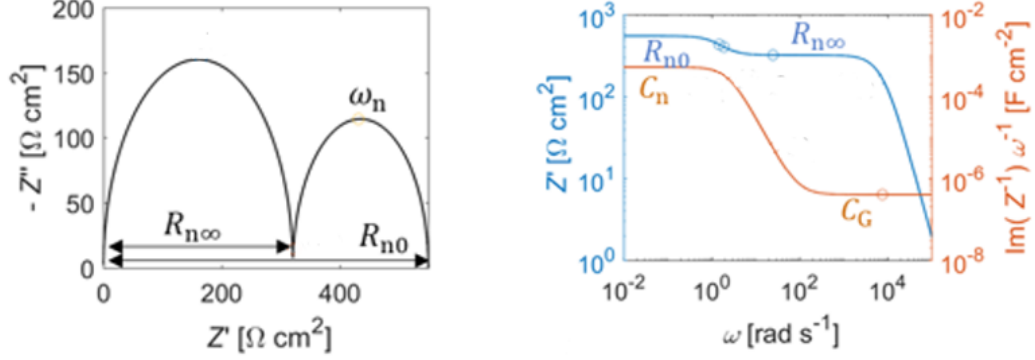


Figure 3: On the left is the Nyquist plot(the real part of total impedance vs. the imaginary part) of the Impedance. On the right is the real part of the impedance and effective capacitance vs. frequency. The important points are circled out in the plots with further explanation in the main text.

guesses can be obtained in the following way.

1. According to the paper,

$$\frac{n_A}{J_n} = R_{n\infty} \frac{q}{k_B T} \quad (1)$$

Therefore,

$$n_A = \frac{J_n R_{n\infty} q}{k_B T} \quad (2)$$

where  $J_n$  can be deduced from the experiment data of  $J$  and light intensity,  $R_{n\infty}$  is read from the plot,  $k_B$  is the Boltzmann constant,  $q$  is the electric constant, and  $T$  is the room temperature (300K by default). In this way, the initial guess of  $n_A$  is obtained.

2. According to the paper,

$$1 - \frac{C_{ion}}{C_A} = k, \quad (3)$$

and

$$C_{ion} = \frac{1}{\omega_n k R_{ion}}, \quad (4)$$

where

$$k = \frac{R_{n\infty}}{R_{n0}}. \quad (5)$$

In equations (3) and (4),  $R_{n\infty}$ ,  $R_{n0}$ , and  $\omega_n$  is read from the plot, and  $R_{ion}$  has to be guessed by the user without a way to be determined directly from the data (the shape of the plot is not very sensitive to the value of  $R_{ion}$  as well). With this information, the initial guesses of  $C_{ion}$  and  $C_A$  can be obtained.

3. According to the paper,

$$J_n = J_s \exp\left(\frac{(V_{A|B} - V_n)q}{n_A k_B T}\right), \quad (6)$$

where  $V_{A|B}$  is the voltage connected to the transistor at the first interface as shown in Fig. 1, and  $V_n$  is the voltage at the right-hand side of the transistor, equal to 0 in this case.

Also, it can be obtained using basic electronics that

$$V_{A|B} = kV \quad (7)$$

at steady state. Therefore,

$$J_s = J_n / \exp\left(\frac{kVq}{n_A k_B T}\right), \quad (8)$$

4. The value of  $C_G$  can be directly used as the initial guess of  $C_g$ . Because at higher frequency, the ionic branch contributes to most of the effective capacitance, so  $C_G = (1/C_g + 1/C_{ion})^{-1}$ . However, the  $C_{ion}$  is much larger than  $C_g$ , so  $C_g$  will contribute mostly to the value of  $C_G$ . Therefore,

$$C_g \approx C_G \quad (9)$$

5. The  $R_s$  will cause a shift of the starting position of the Nyquist plot, so the initial guess of  $R_s$  is taken to be the minimum value of the real part of the impedance. And the initial guess of  $R_{sh}$  is just taken to be a very large value ( $10^5$  by default).

By using the routine illustrated above, a set of initial guesses for parameters  $C_A$ ,  $C_{ion}$ ,  $R_{ion}$ ,  $C_g$ ,  $J_s$ ,  $n_A$ ,  $R_s$ , and  $R_{sh}$  can be obtained.

## 2.2 Individual Fit for 0 Bias Voltage Case

In this scenario, the obtainable initial guesses are different. Specifically, it is impossible to separate  $C_A$  from  $C_{ion}$  and  $J_s/n_A$  can only be obtained together.

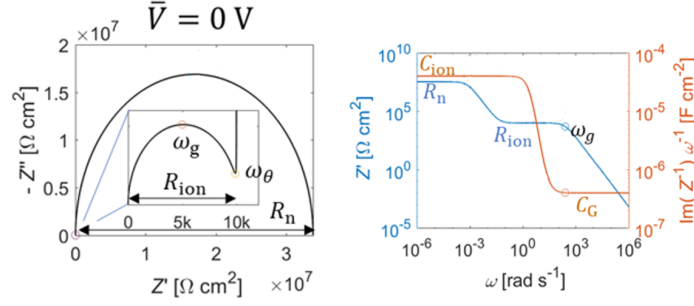


Figure 4: These are the plots for 0 bias voltage. On the left is the Nyquist plot(the real part of total impedance vs. the imaginary part) of the Impedance. On the right is the real part of the impedance and effective capacitance vs. frequency. The important points are circled out in the plots with further explanation in the main text.

Similar to the previous section, the steps for finding the initial guess are:

1.  $R_{ion}$  and  $C_{ion}$  can be directly obtained as shown in the left and right plot respectively.
2. According to the paper,

$$C_g = 1/(R_{ion}\omega_g). \quad (10)$$

where  $\omega_g$  can be obtained from the plot directly.

3. According to the paper,

$$R_n = \frac{k_B T n_A}{q J_s}. \quad (11)$$

Therefore,

$$J_s/n = \frac{k_B T}{R_n q}. \quad (12)$$

where  $R_n$  can be obtained from the plot directly.

4. Also,  $R_n$  is taken as the initial guess for  $R_sh$  and the initial guess of  $R_s$  is obtained in the same way as in the previous section.

By using the routine above, a set of initial guesses for parameters  $C_{ion}$ ,  $C_g$ ,  $R_{ion}$ ,  $J/n_A$ ,  $R_s$  and  $R_{sh}$  can be obtained.

### 2.3 Global Fit Without 0 Bias Voltage

For this case, the tool will use the set of data with the largest bias voltage and find a set of initial guesses using the method of individual non-0 bias voltage cases. However, we assumed in the model that the value of  $C_A$  and  $C_{ion}$  will change with the bias voltage,

$$C(V) = C(0)\sqrt{V_{bi}/(V_{bi} - V_b)}, \quad (13)$$

where  $C$  could be  $C_A$  and  $C_{ion}$ ,  $V_b$  is the bias voltage, and  $V_{bi}$  is the built-in potential of the interface. For the initial guess of the  $V_{bi}$ , it is taken to be 0.2 + maximum bias voltage by rule of thumb, since  $V_{bi}$  has to be bigger than all of the  $V_b$ s.

### 2.4 Global Fit With 0 Bias Voltage

The initial guess finding routine should be nearly the same as global fit without 0 bias voltage. The only difference is, the initial guesses of  $R_{ion}$  and  $R_{sh}$  can be obtained using the same method as in the individual 0 bias voltage case.

### 2.5 Another Method for Finding the initial guesses of $n_A$ and $J_s$ for Global Fit

Starting from eq(8), by taking logarithms on both sides and doing some manipulation,

$$V = n_A k \frac{q}{k_B T} (\log J_n - \log J_s) \quad (14)$$

Therefore, if  $V$  is plotted against  $\log J_n$ , the gradient and the intersect with the x-axis will respectively be,

$$grad = n_A k \frac{q}{k_B T}, \quad (15)$$

and

$$x_0 = -grad \cdot \log(J_s). \quad (16)$$

In this way, for global fitting cases, by plotting the known  $V$ (bias voltage) against known  $J_n$  and doing a linear fit to find the gradient and x intersect, initial guesses of  $n_A$  and  $J_s$  can be obtained correspondingly.