Department of

Electrical & Electronics Engineering

Abdullah Gül University

Project Report of Electrostatic Potential Energy, Infinitely Large Resistor and Capacitor Networks, Wan der Waals bonding, Model for the Resistance in the Cristal Lattice

EE1200 Electronic System Design (ESD) Capsule

Submitted on: 20.05.2023

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OBJECTIVE

The first objective of this study is to derive the analytical series for the electrostatic potential energy between all pairs of ions in an infinite one-dimensional (1D) chain.

The second objective of this study is to perform a numerical evaluation of the Madelung constant α, as defined in Equation (1), for a two-dimensional (2D) infinite NaCl crystal.

The third objective of this study is to investigate the variation of equivalent resistance as the number of nodes increases in a network of resistors representing the electron travel from a Na atom to a Cl atom, or vice versa, in a 2D lattice. By using a simulation tool, a network of resistors with 4, 16, 64, 128, and 256 nodes (each node corresponding to an atom in the lattice) will be formed. The equivalent resistance will be calculated, and the simulation structure and results will be presented in the report. The interpretation of the results will provide insights into how the equivalent resistance changes with an increasing number of nodes in the lattice.

The fifth objective of this study is to construct a resistive network consisting of 4 and 16 nodes using resistors of choice. A test method will be developed to measure the equivalent resistance of the network, and the predictions made in part 3a will be verified in a laboratory environment. The report will explain the test methodology employed for the measurement and include proof of measurements to support the findings.

The fourth objective of this study is to investigate the variation of equivalent capacitance as the number of nodes increases in a network of capacitors representing the effective capacitance between a Na atom and a Cl atom in a 2D lattice. Using a simulation tool, a network of capacitors with 4, 16, 64, 128, and 256 nodes (each node corresponding to an atom in the lattice) will be constructed. The equivalent capacitance will be calculated, and the simulation structure and results will be presented in the report. The interpretation of the results will provide an understanding of how the equivalent capacitance changes with an increasing number of nodes in the lattice.

The sixth objective of this study is to construct a capacitive network using capacitors of choice, with configurations consisting of 4 and 16 nodes. A test method will be developed to measure the equivalent capacitance of the network, and the predictions made in part 4a will be validated in a laboratory environment. The report will detail the test methodology employed for the measurement, including an explanation of the procedures, and provide proof of measurements to support the obtained results.

The seventh objective of this study is to derive analytical equation for the force for the electrostatic potential energy as a function distance r, and to investigate extrema, and find equilibrium for the Lennard-Jones potential

The objective of this analysis is to develop arguments that support the hypothesis that as the temperature decreases, the electrical resistance of the metal decreases, as indicated in Figure 5. By assuming that the magnitude of the black ball oscillations decreases with decreasing temperature, we aim to establish a relationship between the decrease in oscillation magnitude and the decrease in electrical resistance. Furthermore, we seek to explain why we can expect a simple linear plot to describe this relationship.

BACKGROUND

10 ohm resistors, 10uF capacitors, DC source, AC source, soldering, cables, oscilloscope

ANALYTICAL AND SIMULATION PROCEDURES

Part 1 - NaCl Salt Crystal

Let's examine the electrostatic energy of a lattice made up of ions in figure 1. In the case of an ionic crystal such as NaCl, there are positively and negatively charged ions that can be visualized as inflexible spheres. These ions exhibit an electrical attraction until they come into contact. Once in contact, a strong repulsive force arises if any attempt is made to bring them closer together.

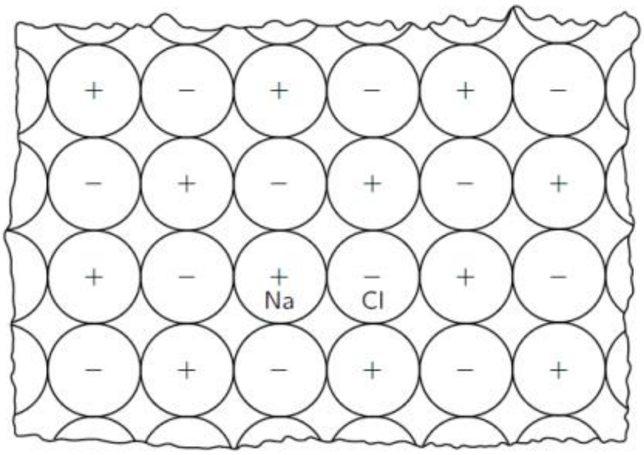

Figure 1 : Lattice demonstration of NaCl crystal

Task 1- The Madelung Constant for 1D Crystal

First we are given an equation for a Na atom as reference point as follows,

$$U = -a.\frac{q^2}{4\pi\varepsilon_0 R_e}$$

- Firstly in order to calculate it let's choose a reference point for our 1D crystal.

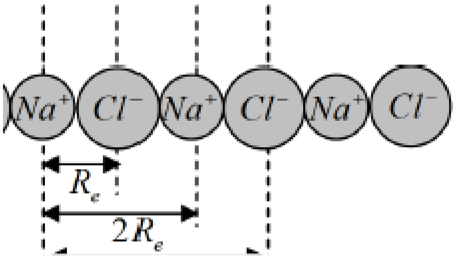

Figure 2 : 1D lattice of NaCl crystal

In the figure Na is our reference point which is located on the left side of the picture

- Secondly we need to calculate the potential energy among for all Na and Cl atom which are located on the right side of our reference point.

Remainder: When we want to calculate the potential energy we use $\frac{q^2}{4\pi\varepsilon Re}$ formula.

1. Potential energy for between Na-Na atoms:

The potential energy between Na and Na atom is $\frac{q^2}{4\pi\varepsilon 2Re}$

But there is one more point that we need to be careful is we need to think about the left side of our reference point , so because of the symmetry we can say

$$U_1{}^1{}_{Na} + U_1{}^2{}_{Na} = \frac{q^2}{4\pi\varepsilon 2Re} + \frac{q^2}{4\pi\varepsilon 2Re} = \frac{2q^2}{4\pi\varepsilon 2Re}$$

Therefore, this is just for the Na-Na potential which has a $2R_e$ distance now lets calculate it for second Na atom.

$$U_2{}^1{}_{Na} + U_2{}^2{}_{Na} = \frac{q^2}{4\pi\varepsilon 4Re} + \frac{q^2}{4\pi\varepsilon 4Re} = \frac{2q^2}{4\pi\varepsilon 4Re}$$

In order to see the geometric series let calculate the Na-Na atoms potential for $6R_e$ distance

$$U_3{}^1{}_{Na} + U_3{}^2{}_{Na} = \frac{q^2}{4\pi\varepsilon 6Re} + \frac{q^2}{4\pi\varepsilon 6Re} = \frac{2q^2}{4\pi\varepsilon 6Re}$$

As you can see we have always $\frac{2q^2}{4\pi\varepsilon}$ constant but our potential changes when our distance changes which is between Na-Na atoms for left and right hand side of our reference points.

2. Potential energy for between Na-Cl atoms:

Now let's look at the potential energy between Na and Cl atoms, while we are calculating the potential energy for our reference point we will consider the left hand side of our reference point again.

So the potential energy between Na and Cl atoms is;

$$U_1{}^1{}_{Cl} + U_1{}^2{}_{Cl} = -\frac{q^2}{4\pi\varepsilon 2Re} - \frac{q^2}{4\pi\varepsilon 2Re} = -\frac{2q^2}{4\pi\varepsilon Re}$$

Therefore, this just for the Na-Cl potential which has a R_e distance now lets calculate it for second Cl atom.

$$U_2{}^1{}_{Cl} + U_2{}^2{}_{Cl} = -\frac{q^2}{4\pi\varepsilon 3Re} - \frac{q^2}{4\pi\varepsilon 3Re} = -\frac{2q^2}{4\pi\varepsilon 3Re}$$

In order to see the geometric series let calculate the Na-Cl atoms potential for $5R_e$ distance

$$U_3{}^1{}_{Cl} + U_3{}^2{}_{Cl} = -\frac{q^2}{4\pi\varepsilon 5Re} - \frac{q^2}{4\pi\varepsilon 5Re} = \frac{2q^2}{-4\pi\varepsilon 5Re}$$

As you can see we have always $-\frac{2q^2}{4\pi\varepsilon}$ constant but our potential changes when our distance changes which is between Na-Cl atoms for left and right hand side of our reference points.

As we found, in order to find the full potential for our reference point we need to collect all results. Then we get:

$$U = -\frac{2q^2}{4\pi\varepsilon Re} + \frac{2q^2}{4\pi\varepsilon 2Re} - \frac{2q^2}{4\pi\varepsilon 3Re} + \frac{2q^2}{4\pi\varepsilon 4Re} - \frac{2q^2}{4\pi\varepsilon 5Re} + \frac{2q^2}{4\pi\varepsilon 6Re} \ldots\ldots\ldots\ldots\ldots$$

We know our $\frac{q^2}{4\pi\varepsilon}$ is a constant number so we can write it as:

$$\frac{q^2}{4\pi\varepsilon}\left[-2\left(1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \frac{1}{6} \ldots \ldots.\right)\right]$$

When we transform into a summations form we get

$$\frac{q^2}{4\pi\varepsilon}(-2).\sum_{n=1}^{\infty}(-1)^{n+1}\left(\frac{x^n}{n}\right)$$

From the given information that is in the question it says electrostatic potential energy U is equal to:

$$U = -a\frac{q^2}{4\pi\varepsilon\mathrm{Re}}$$

We know U so lets put the value instead of U

$$\frac{q^2}{4\pi\varepsilon}(-2).\sum_{n=1}^{\infty}(-1)^{n+1}\left(\frac{x^n}{n}\right) = -a\frac{q^2}{4\pi\varepsilon\mathrm{Re}}$$

When we make the simplification between the equations we get the **Madelung Constant** as:

$$-a = (-2).\sum_{n=1}^{\infty}(-1)^{n+1}\left(\frac{x^n}{n}\right)$$

$$so\ a\ is:$$

$$a = (2).\sum_{n=1}^{\infty}(-1)^{n+1}\left(\frac{x^n}{n}\right)$$

- Thirdly to find the function of a **Madelung Constant** first we need to transform our summation to Alternating harmonic series:

$$y(x) = \sum_{n=1}^{\infty}(-1)^{n+1}\left(\frac{x^n}{n}\right)$$

We need to find x=1 for Alternating Harmonic series

$$y(1) = \sum_{n=1}^{\infty}(-1)^{n+1}n^{-1}$$
$$= 1 - \frac{1}{2} + \frac{1}{3} \dots$$

So f(x) is equal to

$$f(x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \frac{x^5}{5} - \frac{x^6}{6} \dots.$$

Now lets take the derivative of f(x)

$$f'(x) = 1 - x + x^2 - x^3 + x^4 \dots.$$

Then collect positive and negative sides in one part we get

$$1 + x^2 + x^4 + x^6 \ldots . -x(1 + x^2 + x^4 + x^6 \ldots . .)$$

We know that

$$\frac{1}{1-x} = 1 + x + x^2 + x^3 \ldots$$

So we get,

$$\text{f'}(x) = \frac{1}{1-x^2} - x . \frac{1}{1-x^2}$$

If we arrange this, we get

$$\text{f'}(x) = \frac{1}{1+x}$$

When we take the integral of both side we will get the f(x)

$$\int \text{f'}(x)dx = \int \frac{1}{1+x}dx$$

$$f(x) = \ln(1+x) + c$$

We know f(0)=0 so c=o that means f(x) is equal to

$$f(x) = \ln(1+x)$$

We were looking for f(1) so

f(1) = ln2

So as a result our Madelung Constant for 1D lattice is

$$a = 2ln2$$

Task 2- The Madelung Constant for 2D Crystal

For this part we are going to make numerical analysis of the Madelung Constant from equation $U = -a . \frac{q^2}{4\pi\varepsilon_0 \text{R}_e}$ in 2D lattice.

First we choose a reference Na atom in 2D lattice,

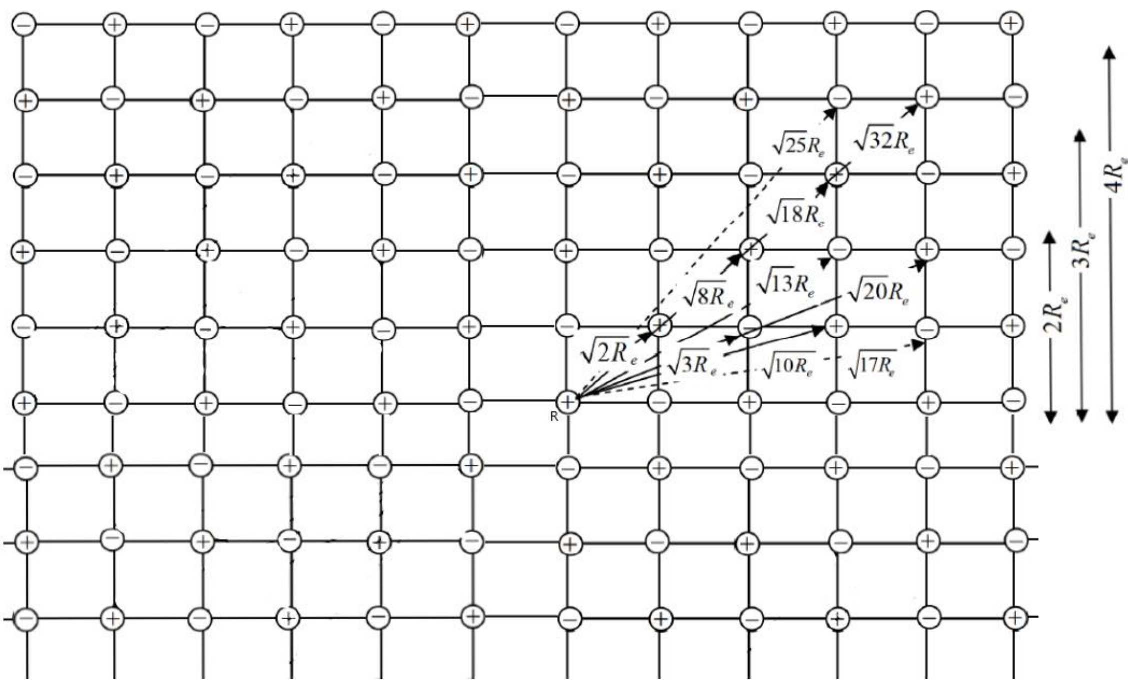

Figure 3 : 2D lattice of NaCl crystal

First we write the electrostatic potential energy of reference Na atom with 8 in 3x3 others which surrounds reference,

$$4*\frac{-q^2}{4\pi\varepsilon_0 R_e}+4*\frac{q^2}{4\pi\varepsilon_0\sqrt{2}R_e}+8*\frac{-q^2}{4\pi\varepsilon_0\sqrt{5}R_e}+4*\frac{q^2}{4\pi\varepsilon_0 2R_e}+4*\frac{q^2}{4\pi\varepsilon_0 2\sqrt{2}R_e}$$

All in common is $\frac{q^2}{4\pi\varepsilon_0 R_e}$, take the parentheses, we have,

$$4-\frac{4}{\sqrt{2}}+2-\frac{8}{\sqrt{5}}-\frac{4}{2\sqrt{2}}+\frac{4}{3}-\frac{4}{3\sqrt{2}}+\frac{8}{\sqrt{13}}-\frac{8}{\sqrt{10}}-\frac{4}{4}\ldots.=a$$

As a result, constant converges around 1.61

Task 3a- Equivalent resistance of infinitely large resistor networks.

Given the network of NaCl crystal, let us think that every ions are nodes and every way between nodes are resistors with r0,

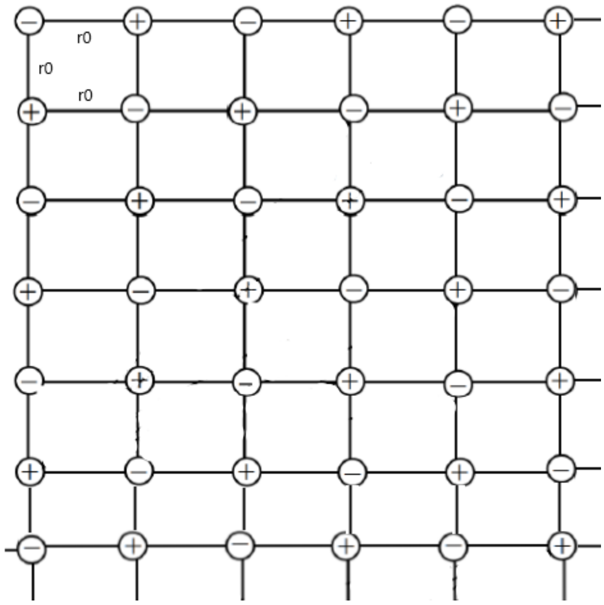

Figure 4 : 2D lattice of NaCl for resistance networks

The task asks us to create a network in SPICE with 4, 16, 64, 128 and 256 nodes, and to calculate equivalent resistance. We use the method of using Ohm’s Law to measure equivalent resistance. So we apply voltage through the network, and we get a current value, so from the equation V=IR, we can calculate the resistance.We used Protues for SPICE simulation, and we crated networks with 10 ohms resistors and 1 V DC source as follows,

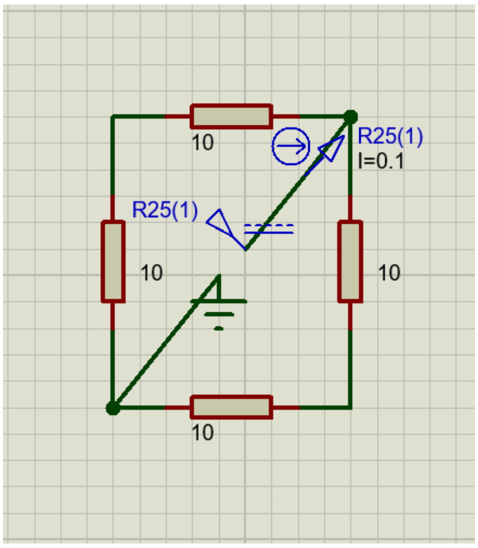

Figure 5 : Resistance network with 4 nodes

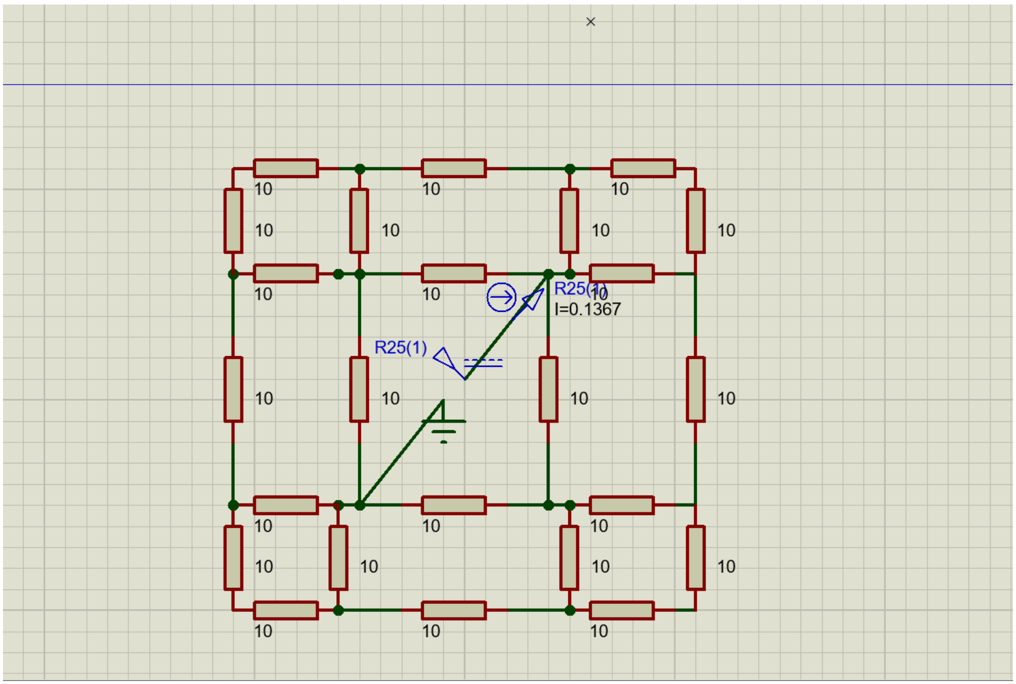

Figure 6 : Resistance network with 16 nodes

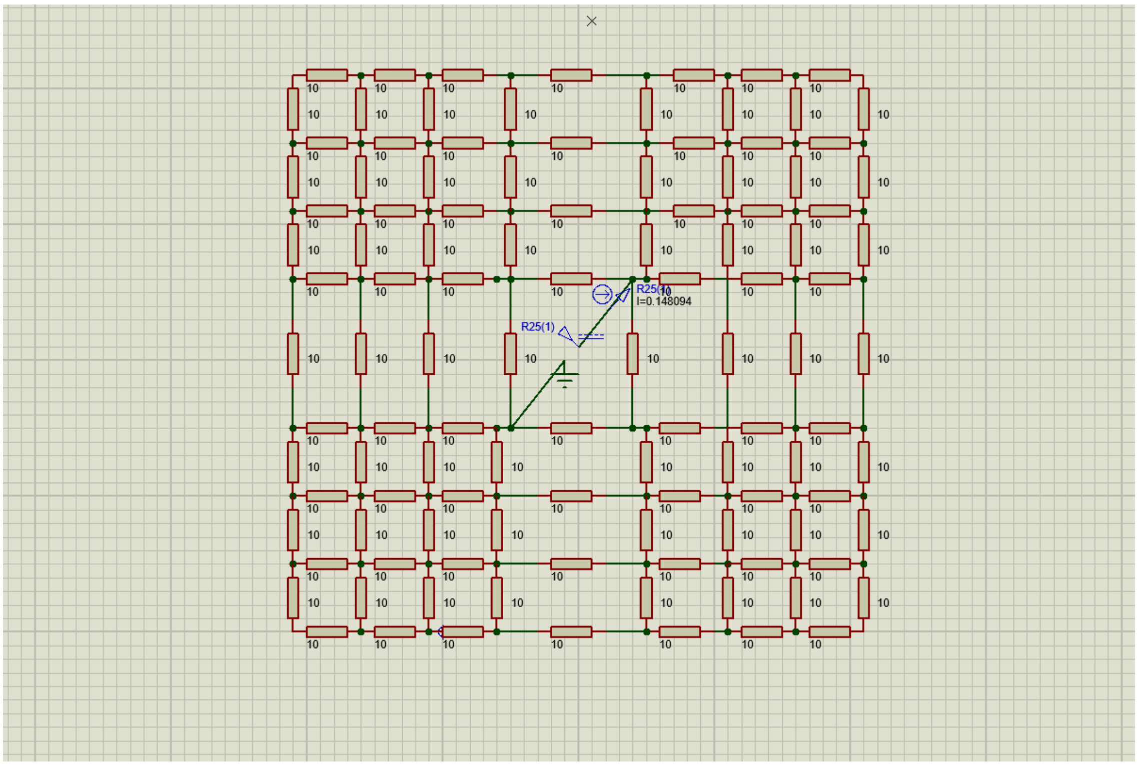

Figure 7 : Resistance network with 64 nodes

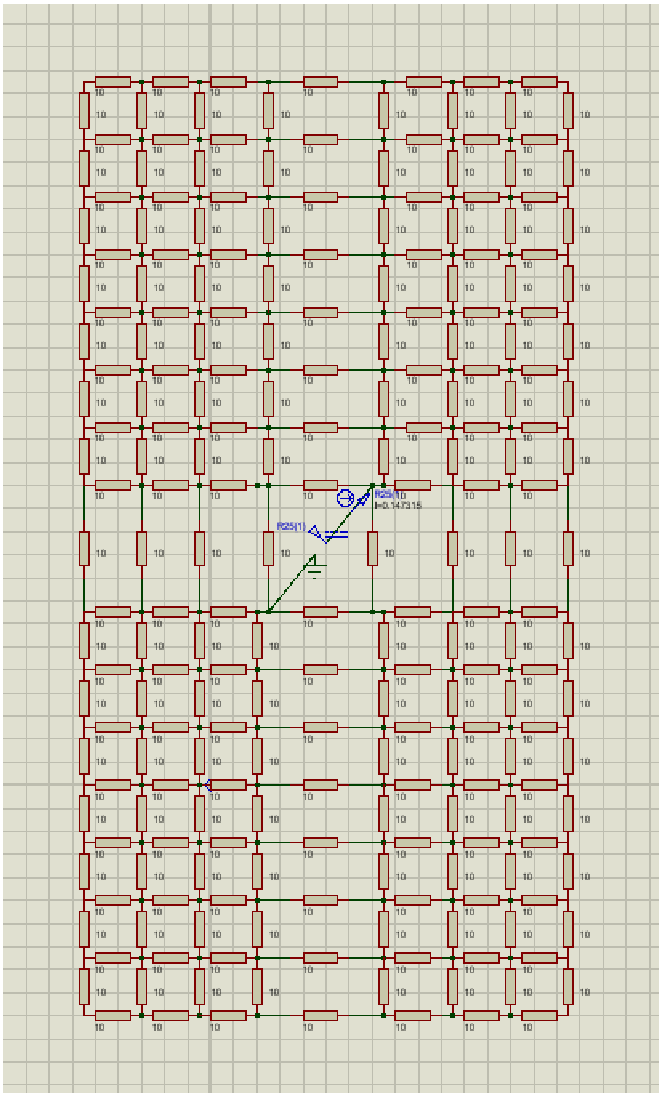

Figure 8 : Resistance network with 128 nodes

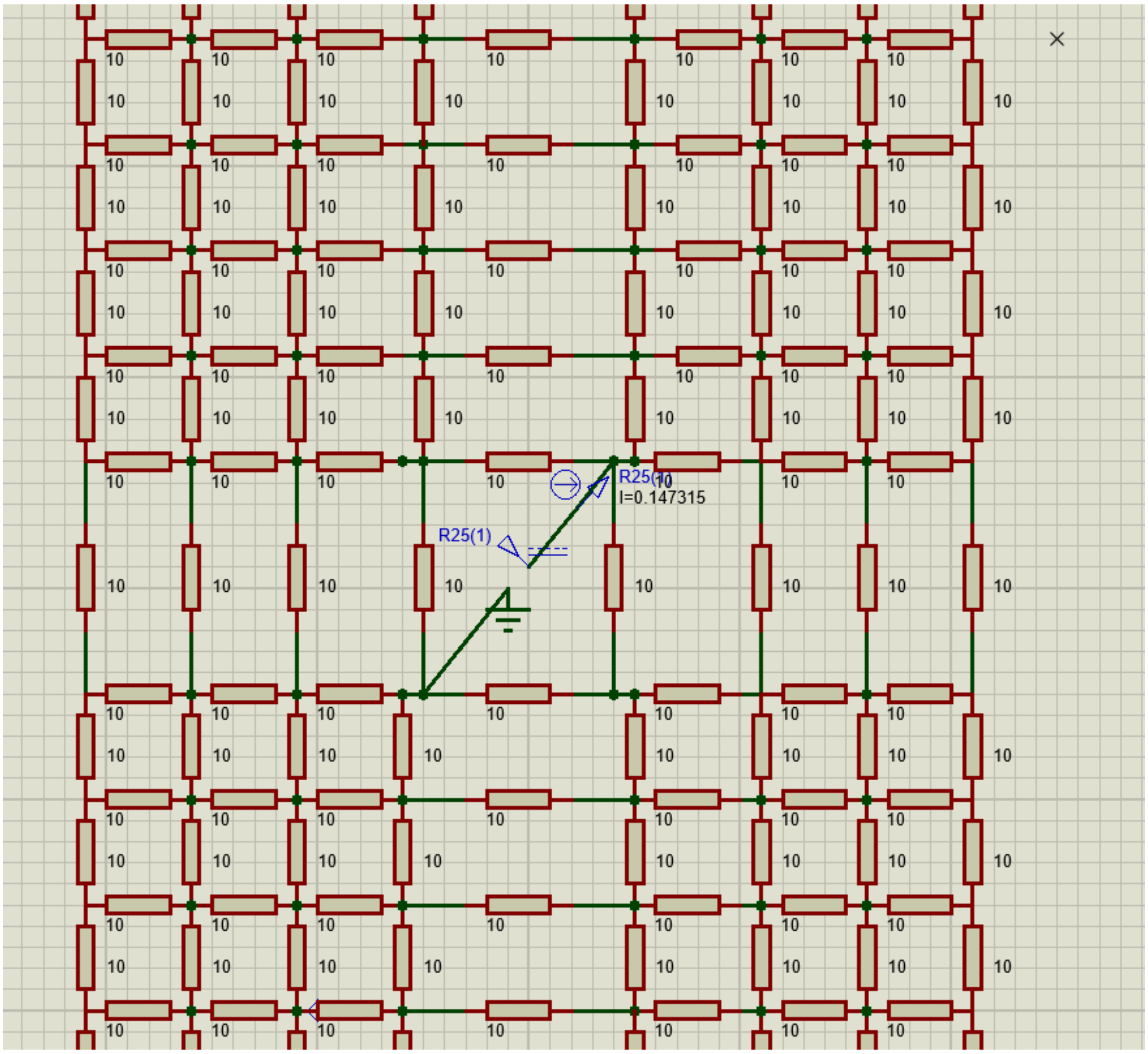

Figure 9 : Resistance network with 128 nodes with a close view

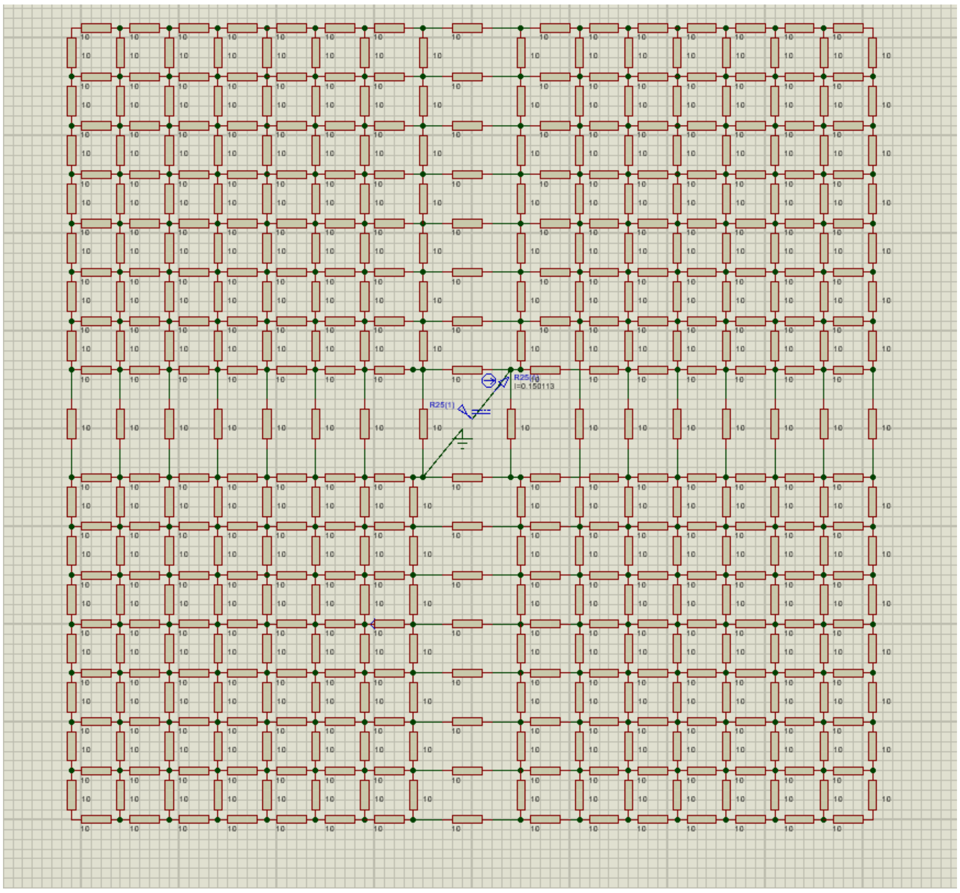

Figure 10 : Resistance network with 64 nodes

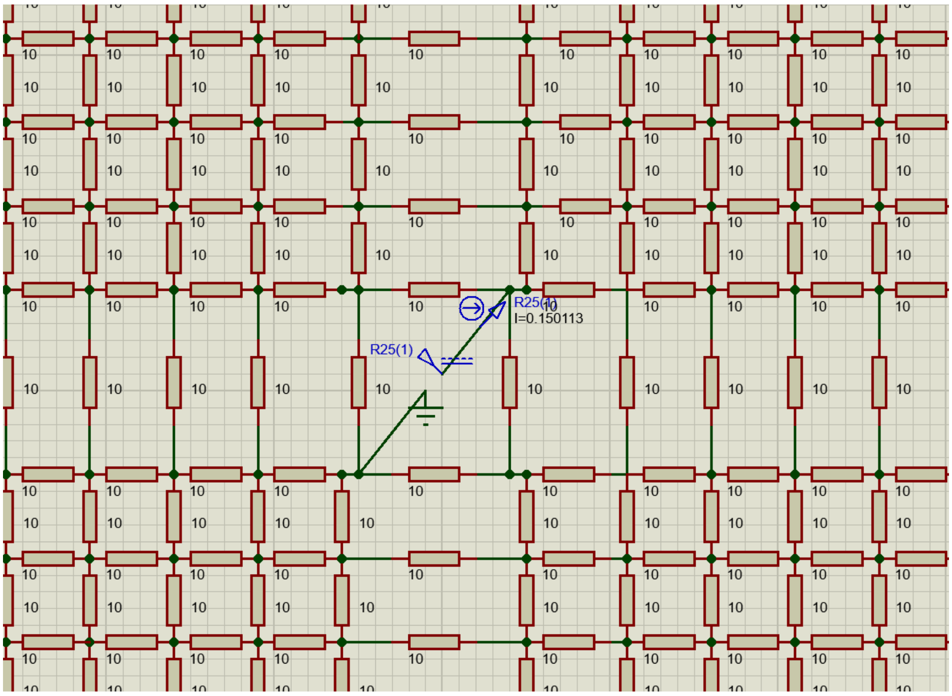

Figure 11 : Resistance network with 64 nodes with a close view

So from our network systems, we can make a comment on equivalent resistance values by using Ohm’s Law.

Number of Nodes	Voltage	Current	Equivalent Resistance of Network
4	1 V	0.1 A	10 Ω
16	1 V	0.1367 A	7,315288 Ω
64	1 V	0.14096 A	7,09421 Ω
128	1 V	0.147315 A	6,78817 Ω
256	1 V	0.150113 A	6,66164 Ω

Task 3b- Equivalent resistance of infinitely large resistor networks in Lab environment.

For this part, by soldering resistors we created a network of resistors with 10 ohms in the lab environment. Then, as we did in the task 3a, we used the method of applying voltage through the network, and we got current values. So our results are as follows,

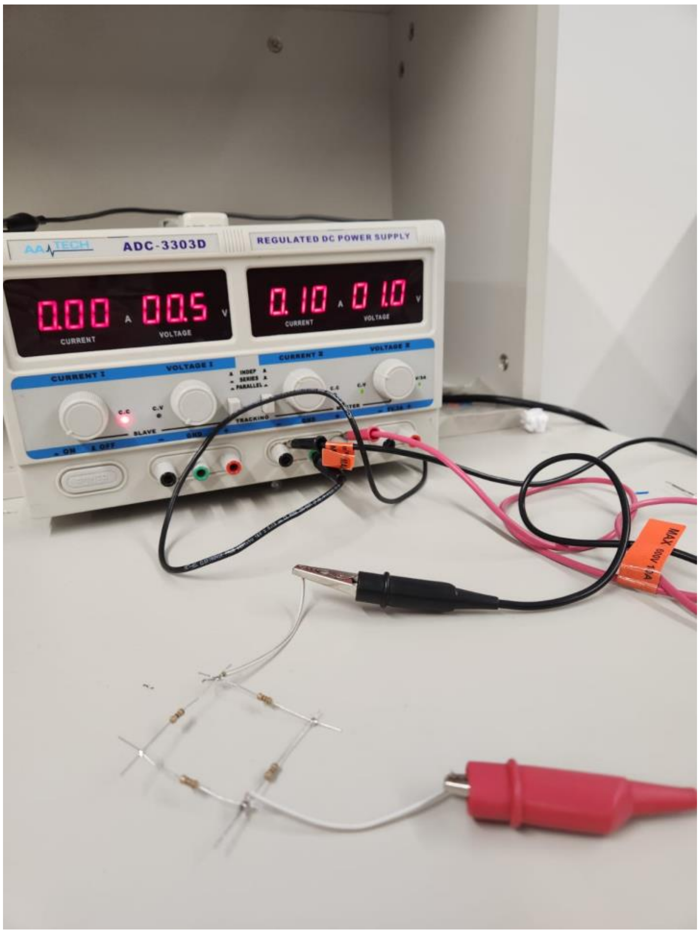

Figure 12 : Lab experiment for 4 nodes network

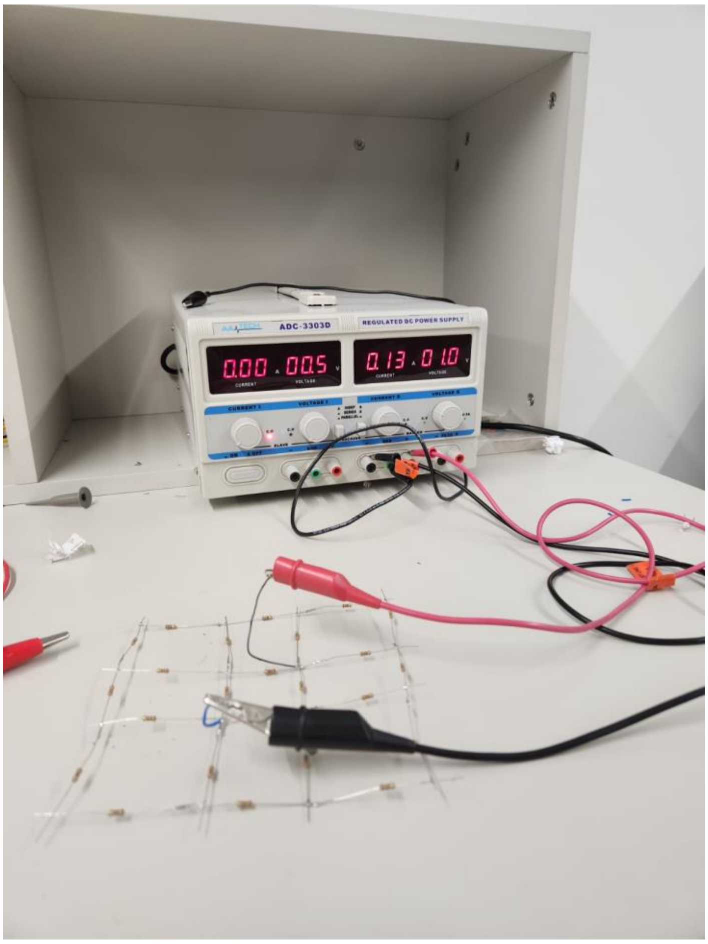

Figure 13 : Lab experiment for 16 nodes network

So from our network systems, we can make a comment on equivalent resistance values by using Ohm's Law.

Number of Nodes	Voltage	Current	Equivalent Resistance of Network
4	1 V	0.1 A	10 Ω
16	1 V	0.13 A	7,69230 Ω

Task 4a- Equivalent capacitance of infinitely large capacitor networks

Given the network of NaCl crystal, let us think that every ions are nodes and every way between nodes are capacitors with C,

The task asks us to create a network in SPICE with 4, 16, 64, 128 and 256 nodes, and to calculate equivalent capacitance. We use the method of observation of transient analysis to measure equivalent capacitance. So we apply voltage through the network, we get a step response then we observe the voltage across the resistance which is connected in series to circuit

We used Protues for SPICE simulation, and we crated networks with 10µF capacitors and 100 V DC and 10 ohm resistor.

First let us look at 4 nodes network,

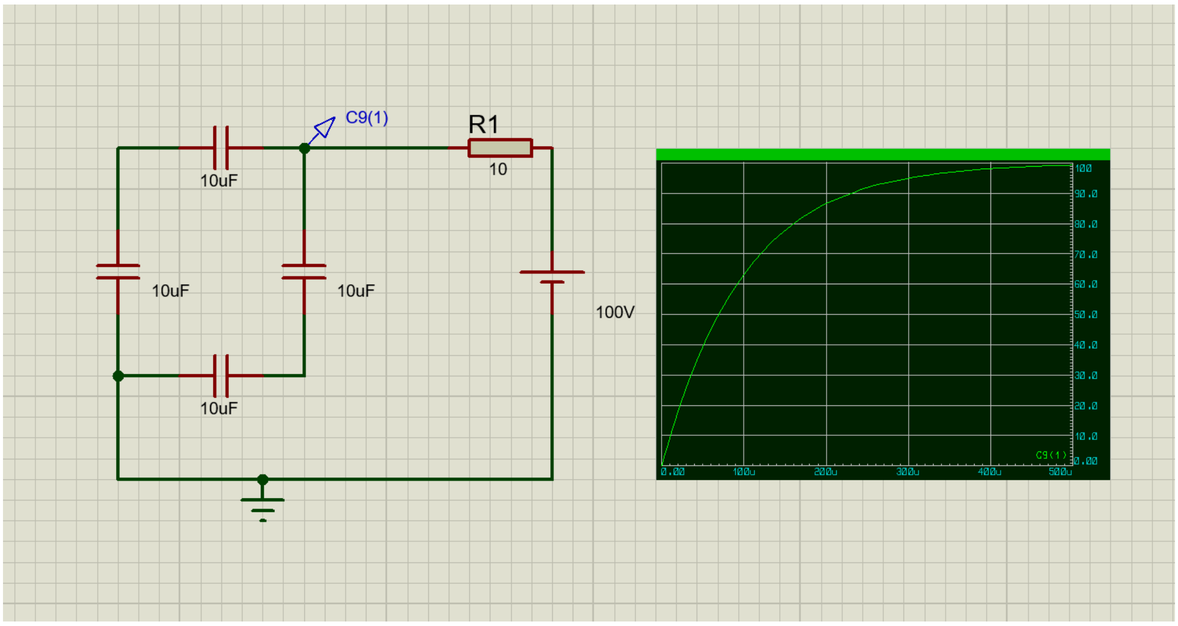

Figure 14 : Capacitor network for 4 nodes and its graph of transient analysis

We created the given above circuit, then we observe the transient analysis. Before moving into this, we should remember that step response of this circuit.

We already know that voltage across the resistor,

$$V(t) = v(\infty) + [v(0) - v(\infty)]e^{-\frac{t}{\tau}}$$

Where is $v(0) = 0$and $v(\infty) = 100$, and our time constant $(\tau = RC)$ is 10C

$$V(t) = 100 - 100e^{-\frac{t}{\tau}}$$

We know that observed time taken for the voltage across the resistor to reach approximately 63.2% of its maximum value during the charging or discharging phase and this value 63.2% is nearly 1 τ. So 63.2% of its maximum value is 63.2 V. We tracked this value from the graph, given below

Figure 15 : The graph of transient analysis of 4 nodes network

From the graph of transient analysis, we can see that voltage reaches 63.2 V in 99.9u second(0.0000999 second). So we can calculate equivalent capacitance by using this formula

$$V(t) = 100 - 100e^{-\frac{t}{\tau}}$$

So if we put numbers in we get,

$$63.2 \; = 100 - 100e^{-\frac{0.0000999}{\tau}}$$

$$36.8 \; = 100e^{-\frac{0.0000999}{\tau}}$$

$$e^{-\frac{0.0000999}{\tau}} = 0{,}368$$

Our time constant is 10C

$$e^{-\frac{0.0000999}{10C}} = 0{,}368$$

Take ln both sides,

$$-\frac{0.0000999}{10C} = -0{,}9996$$

$$-\frac{0.0000999}{10(-0{,}9996)} = C$$

As a result, equivalent capacitance C is 9,99uF, so it is nearly 10µF.

For the circuit having 16 nodes, again we used a voltage source having 100V and resistor having 10

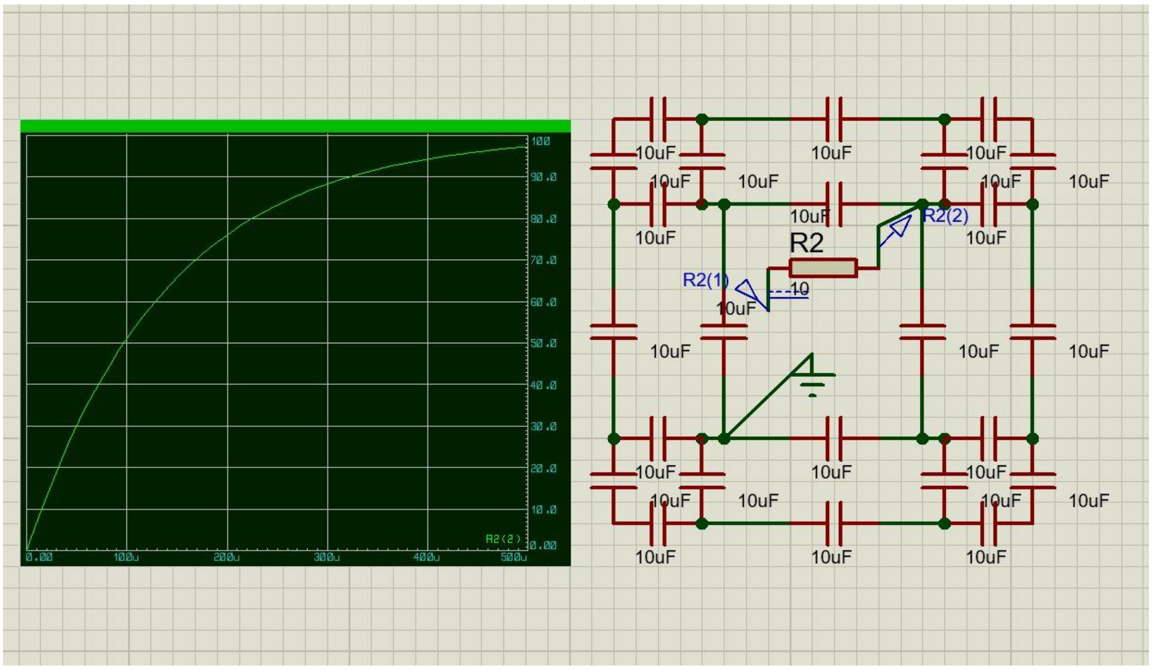

Figure 16 : Capacitor network for 16 nodes and its graph of transient analysis

Ω.

Again, the formula for the circuit:

$$V(t) = 100 - 100e^{-\frac{t}{\tau}}$$

In Proteus, we observed the time from the graph of transient analysis given below.

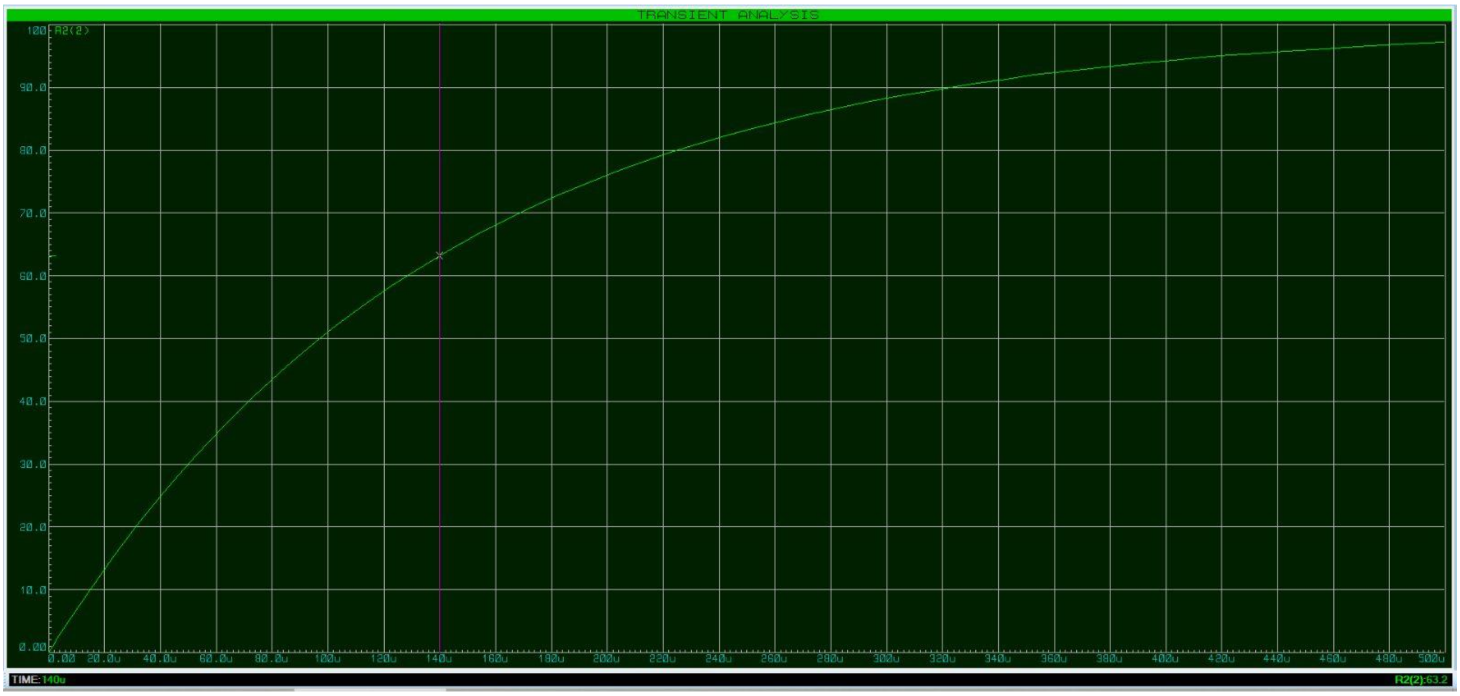

Figure 17 : The graph of transient analysis of 16 nodes network

t = 140u (0.00014 second) So, the voltage reaches 63.2 V in 0.00014 second.

$$V(t) = 100 - 100e^{-\frac{t}{\tau}}$$

$$63.2 = 100 - 100e^{-\frac{0.00014}{\tau}}$$

$$36.8 \ = 100e^{-\frac{0.00014}{\tau}}$$

$$e^{-\frac{0.00014}{\tau}} = 0{,}368$$

In this circuit, $\tau = 10C$ too which is the same for all circuits because we have one resistor having 10 Ω.

$$e^{-\frac{0.00014}{10C}} = 0{,}368$$

Take ln both sides,

$$-\frac{0.00014}{10C} = -0{,}9996$$

$$C = \frac{0.00014}{10 * (0{,}9996)}$$

$$C = 14\text{uF}$$

For the circuit having 64 nodes:

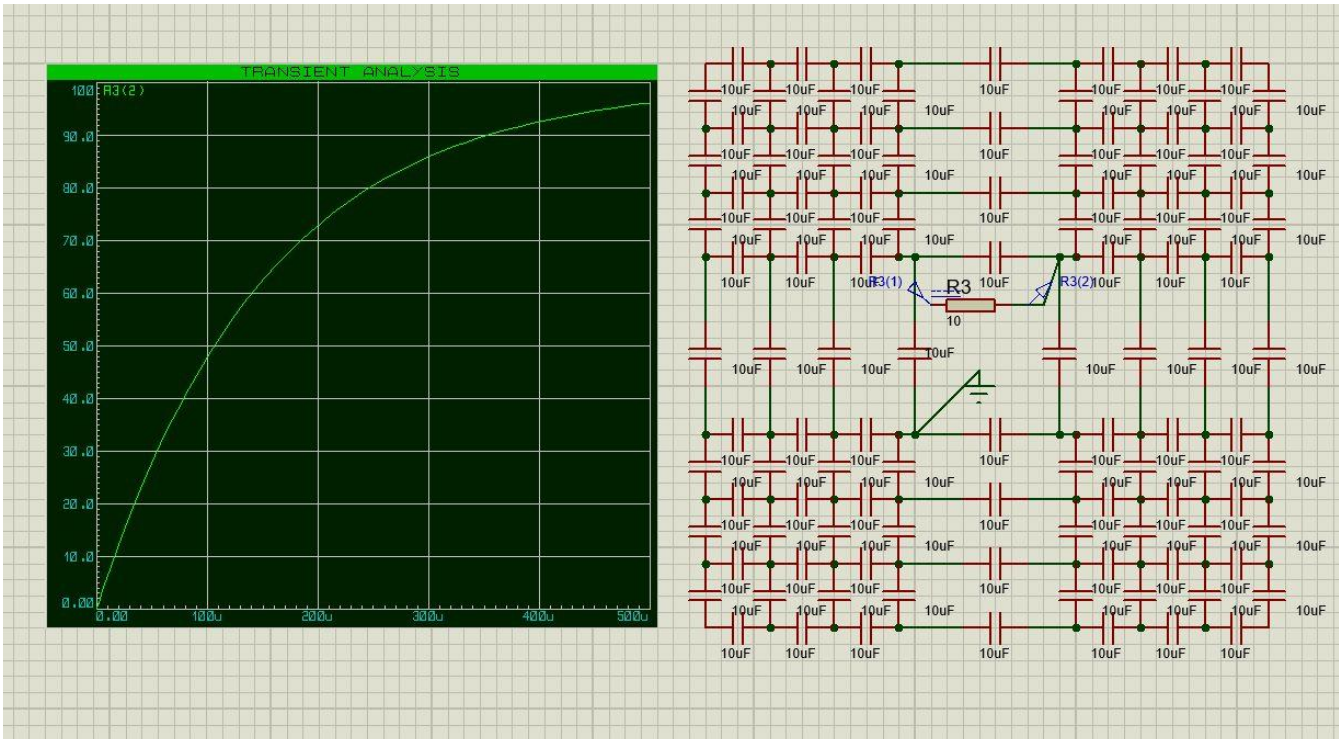

Figure 18 : Capacitor network for 64 nodes and its graph of transient analysis

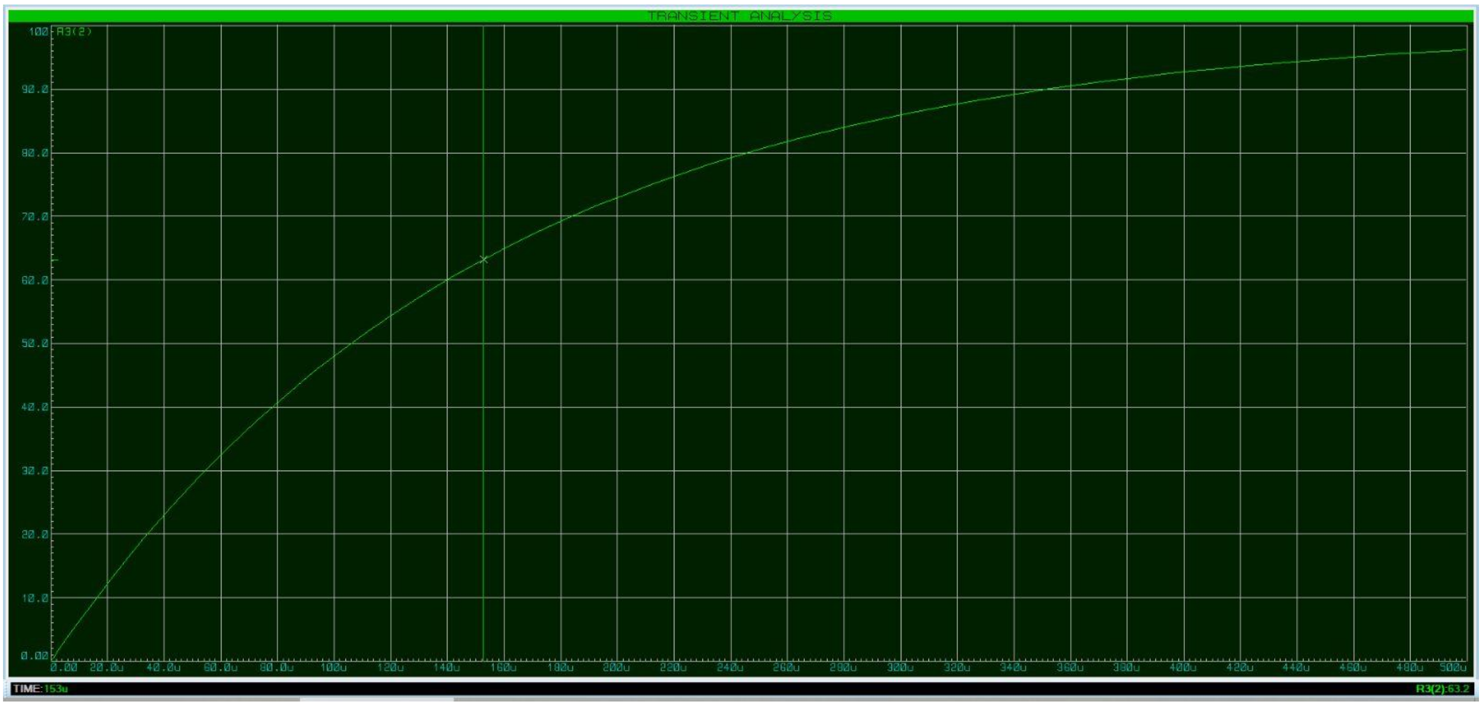

Figure 19 : The graph of transient analysis of 64 nodes network

As we can see from the graph of transient analysis, our t value equals to 153u (0.000153 second).

$$V(t) = 100 - 100e^{-\frac{t}{\tau}}$$

$$63.2 = 100 - 100e^{-\frac{0.000153}{\tau}}$$

$$36.8 \ = 100e^{-\frac{0.000153}{\tau}}$$

$$e^{-\frac{0.000153}{\tau}} = 0{,}368$$

$$e^{-\frac{0.000153}{10C}} = 0{,}368$$

Take ln both sides,

$$-\frac{0.000153}{10C} = -0.9996$$

$$C = \frac{0.000153}{10 * (0.9996)}$$

$$C = 15.3\ u\text{F}$$

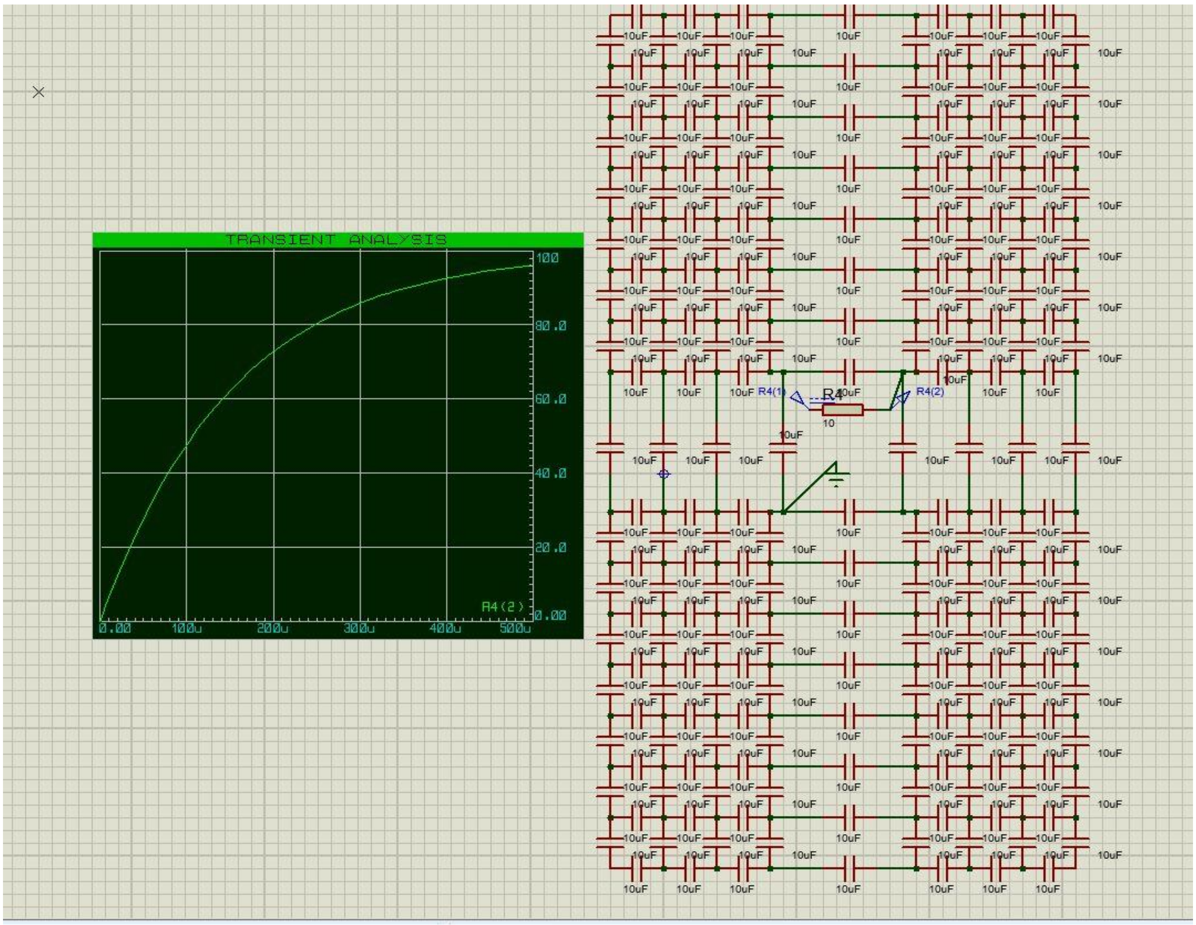

Figure 20 : Capacitor network for 128 nodes and its graph of transient analysis

For the circuit having 128 nodes:

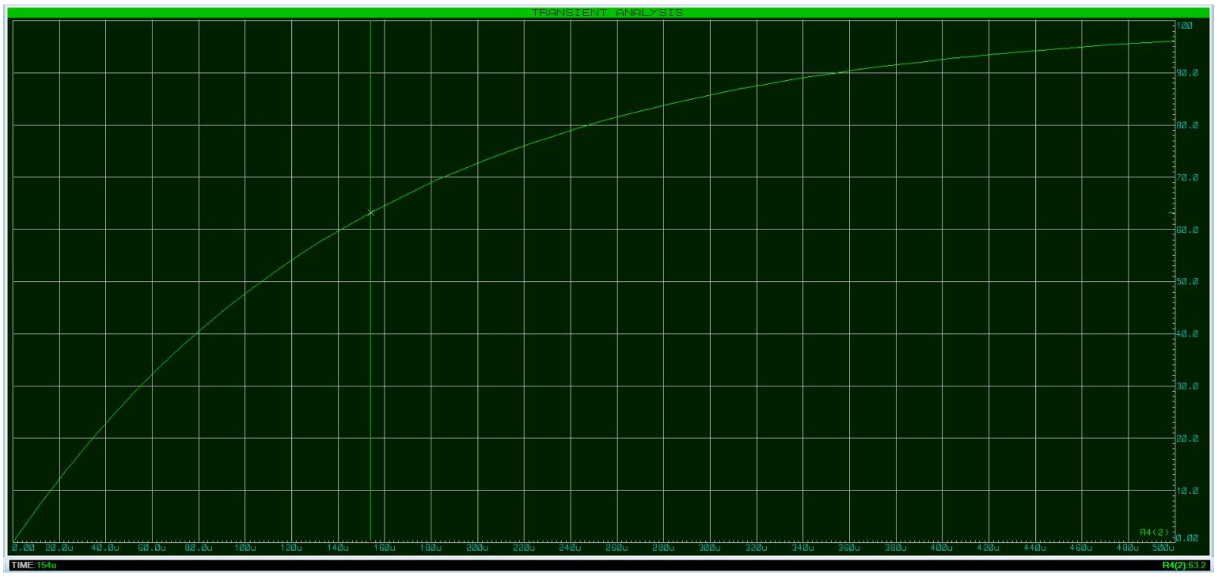

Figure 21 : The graph of transient analysis of 128 nodes network

In this network, our t value equals to 154u (0.000154 second).

$$V(t) = 100 - 100e^{-\frac{t}{\tau}}$$

$$63.2 = 100 - 100e^{-\frac{0.000154}{\tau}}$$

$$36.8 \;= 100e^{-\frac{0.000154}{\tau}}$$

$$e^{-\frac{0.000154}{\tau}} = 0{,}368$$

$$e^{-\frac{0.000153}{10C}} = 0{,}368$$

Take ln both sides,

$$-\frac{0.000154}{10C} = -0{,}9996$$

$$C = \frac{0.000154}{10 * (0{,}9996)}$$

$$c = 15.4\, uF$$

For the circuit having 256 nodes:

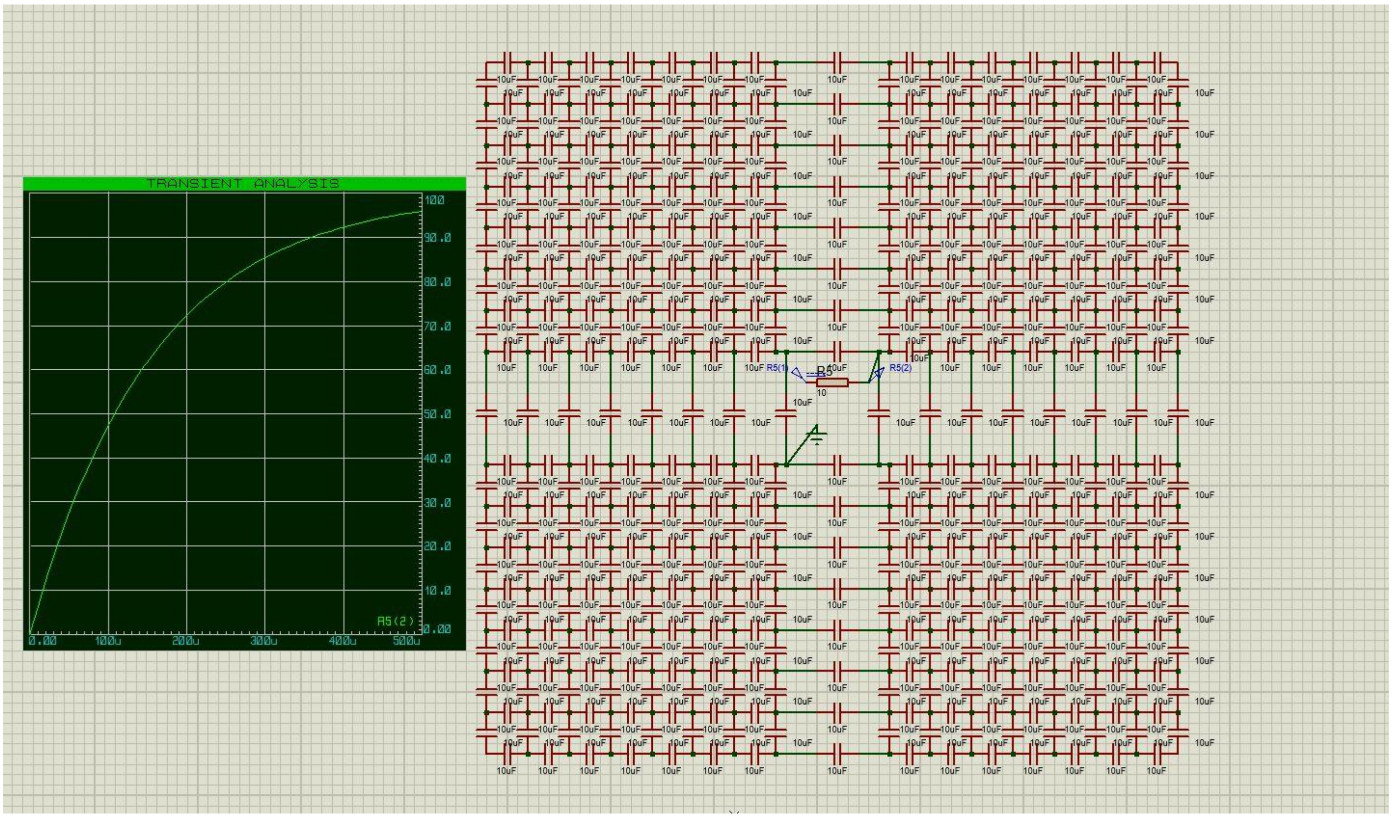

Figure 22 : Capacitor network for 256 nodes and its graph of transient analysis

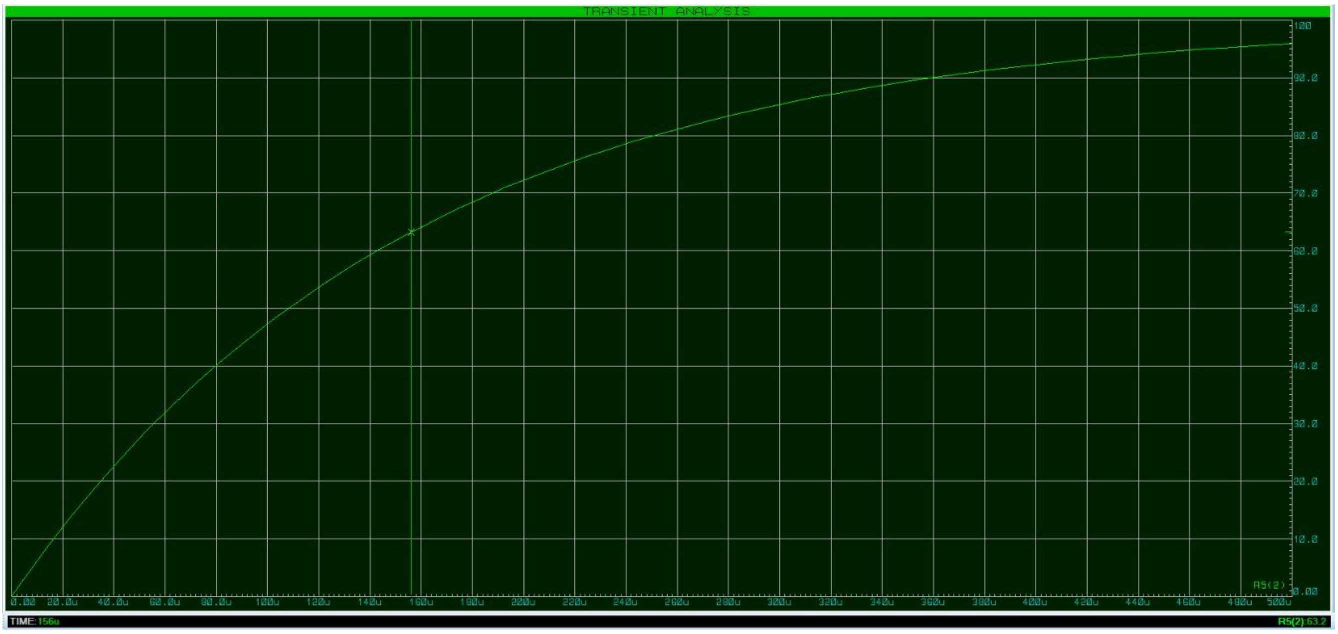

Figure 23 : The graph of transient analysis of 256 nodes network

In this network, t = 156u (0.000156 second).

$$V(t) = 100 - 100e^{-\frac{t}{\tau}}$$

$$63.2 = 100 - 100e^{-\frac{0.000156}{\tau}}$$

$$36.8 \; = 100e^{-\frac{0.000156}{\tau}}$$

$$e^{-\frac{0.000156}{\tau}} = 0{,}368$$

$$e^{-\frac{0.000156}{10C}} = 0{,}368$$

Take ln both sides,

$$-\frac{0.000156}{10C} = -0{,}9996$$

$$C = \frac{0.000156}{10 * (0{,}9996)}$$

$$C = 15.6\, uF$$

We can see from the table the difference of these circuit's equivalent capacitance:

Number of nodes	τ	t	Equivalent Capacitance of Network
4	10C	0.0000999 second	10uF
16	10C	0.00014 second	14uF
64	10C	0.000153 second	15.3uF
128	10C	0.000154 second	15.4uF
256	10C	0.000156 second	15.6uF

Task 4b- Equivalent capacitance of infinitely large capacitor networks in lab environment

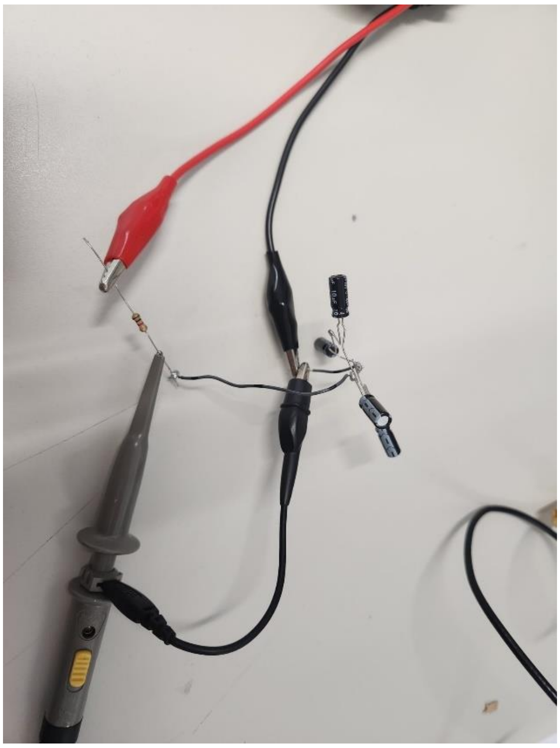

Figure 24: Circuit design for 4 nodes network

We created the given above circuit with 4 nodes, 10uF and 1K resistor and time constant 1000C, then we observed the transient analysis. Before moving into this, we should remember that step response of this circuit.

We already know that voltage across the resistor,

$$V(t) = v(\infty) + [v(0) - v(\infty)]e^{-\frac{t}{\tau}}$$

We used signal generator to generate square sign, from 0 to 2V with 10Hz, then our formula becomes this,

Figure 25: The properties of square signal that is used for calculating capacitance of 4 nodes network

$$V(t) = 2 + [v(0) - 2]e^{-\frac{\Delta t}{1000C}}$$

To calculate the equivalent capacitance, we used oscilloscope to measure Δt and $v(0)$, by using cursors.

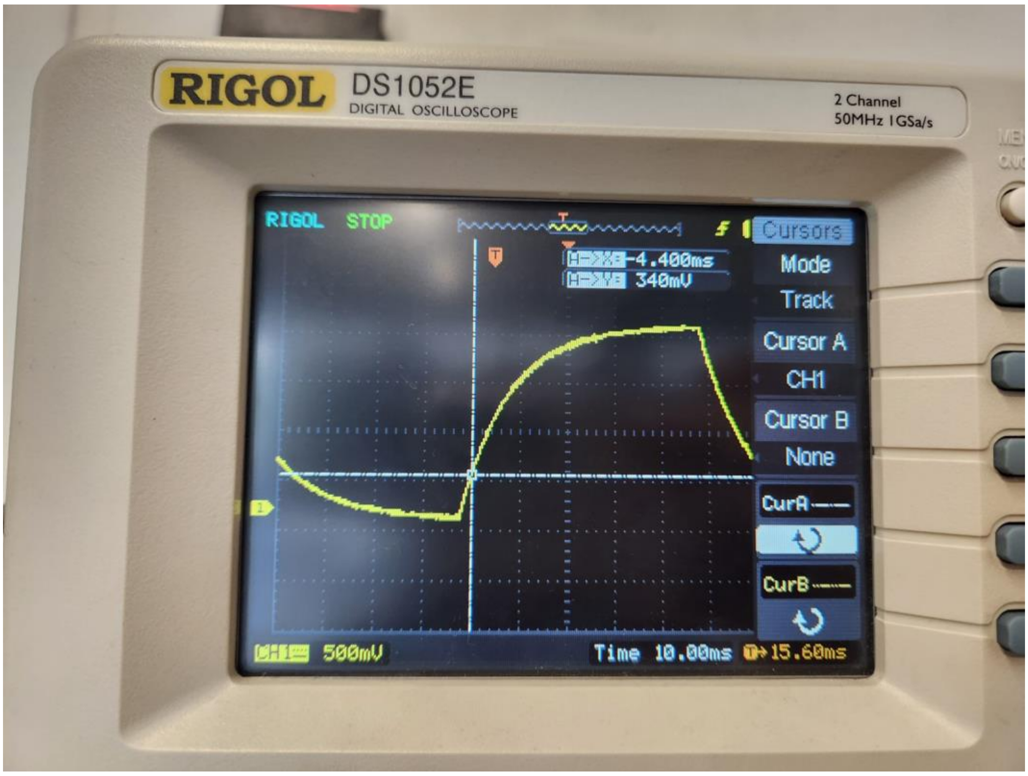

Figure 26: Oscilloscope result for 4 nodes network

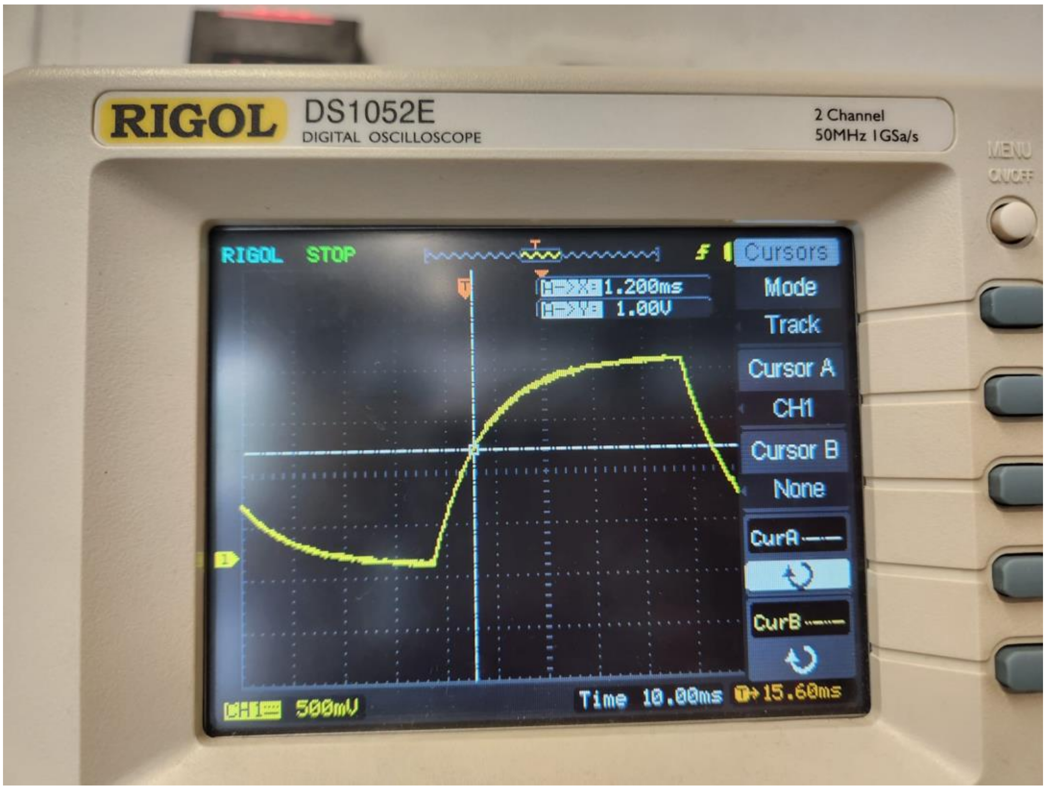

Figure 27: Oscilloscope result for 4 nodes network

From given above pictures, our $v(0)$ value is 0.340 V, and our Δt value is 5.6ms, and also capacitor voltage reaches to 1V. If we put these numbers into the equation, we get,

$$1 = 2 + [0.340 \ - 2]e^{-\frac{0,0056}{1000C}}$$

Then the rest is calculation,

$$-1 = [-1.66]e^{-\frac{0,0056}{1000C}}$$

$$0,602409 = e^{-\frac{0,0056}{1000C}}$$

$$-0,506818 = -\frac{0,0056}{1000C}$$

Then our equivalent capacitance is 11.49 uF. It is close to the value that we found in simulation.

For the second experiment with the network having 16 nodes, we used the same square signal and same resistor.

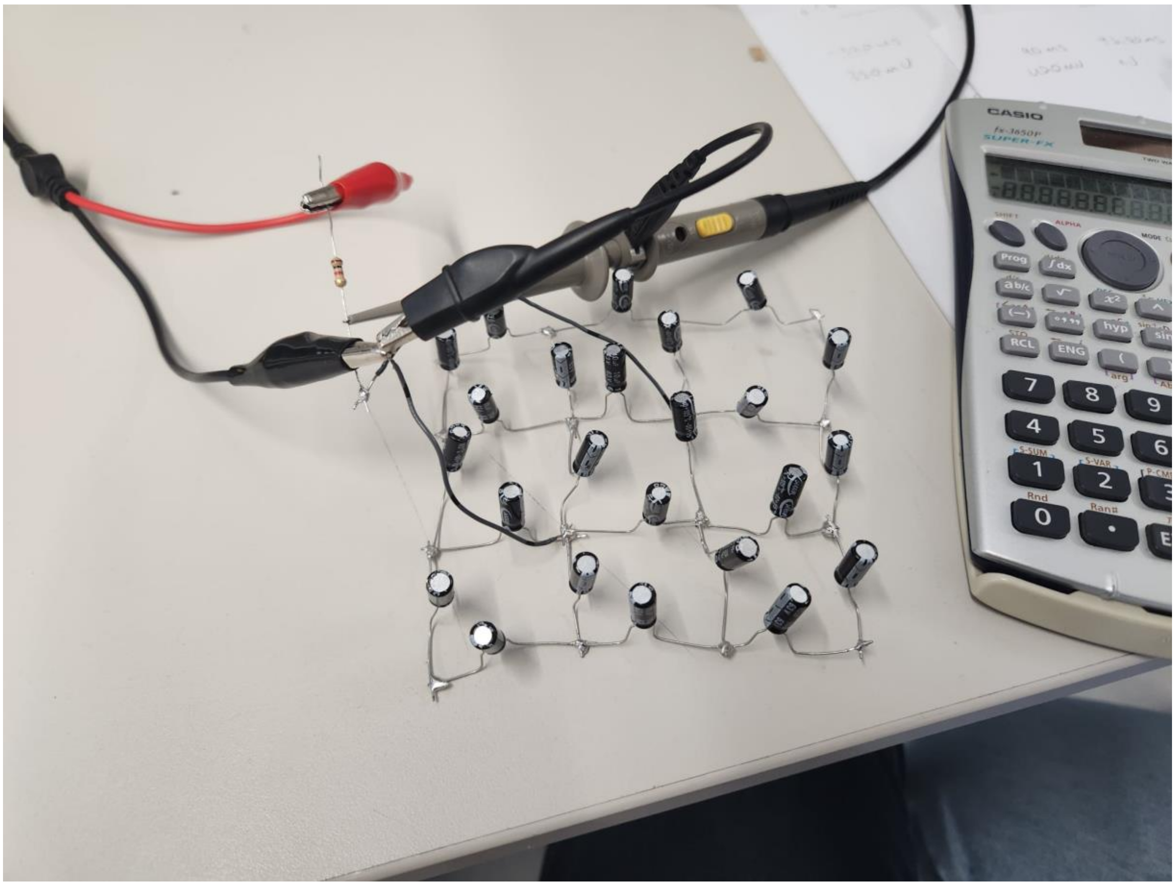

Figure 28: Circuit design for 16 nodes network

And our oscilloscope results are as follows,

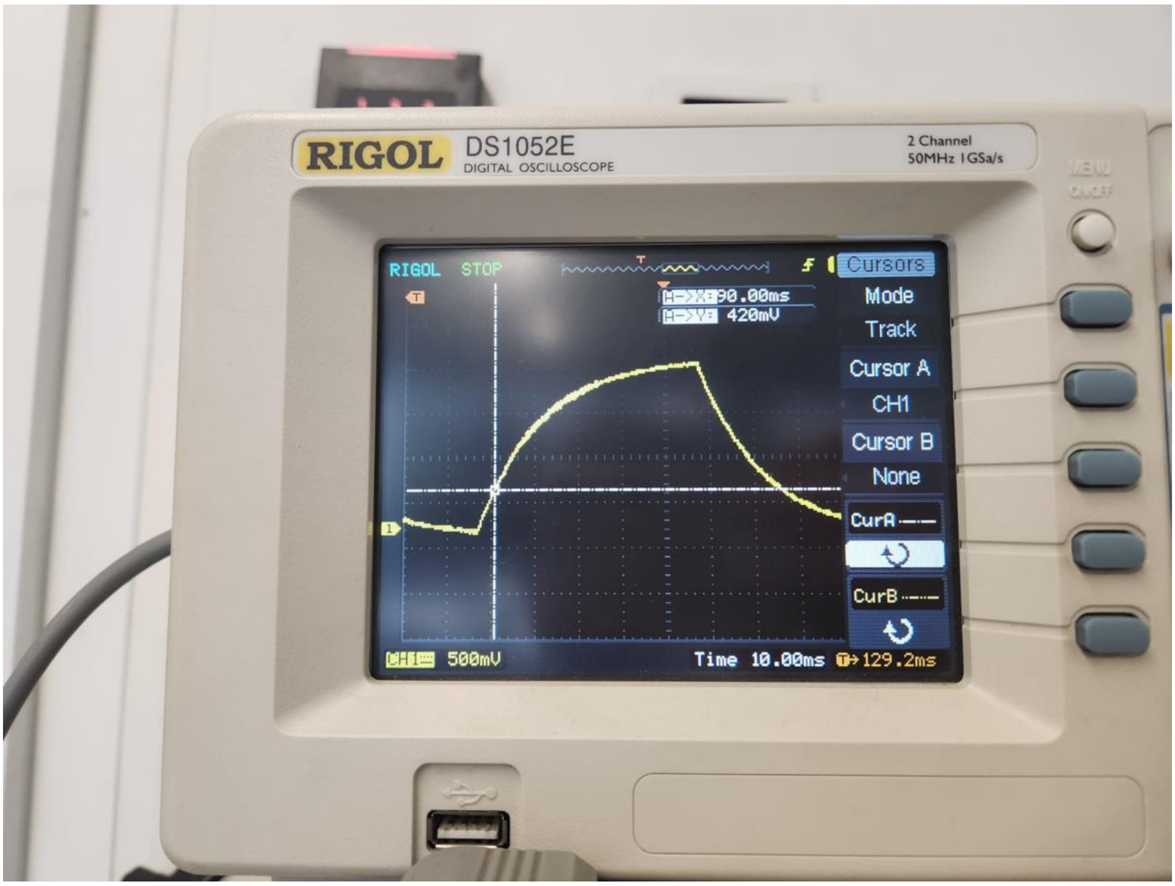

Figure 29: Oscilloscope result for 16 nodes network

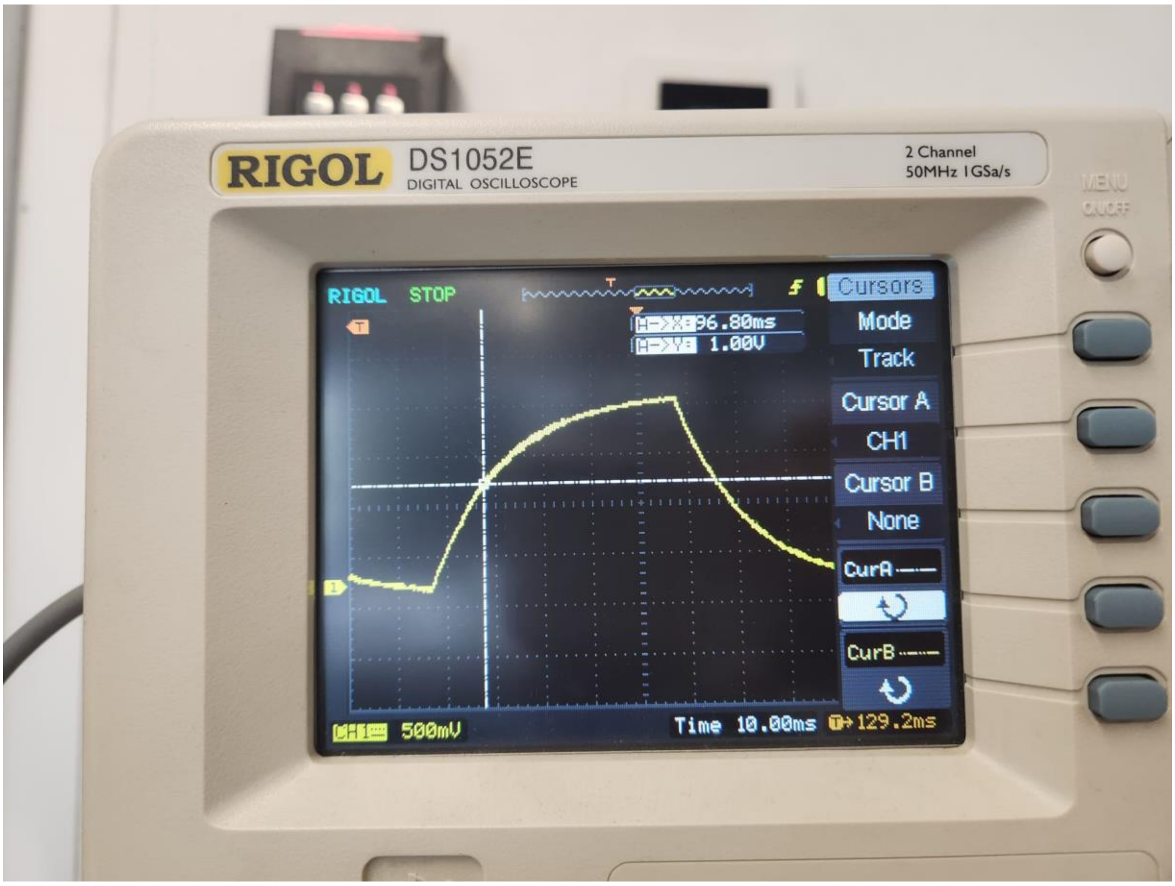

Figure 30: Oscilloscope result for 16 nodes network

From given above pictures, our $v(0)$ value is 0.420 V, and our Δt value is 6.80ms, and also capacitor voltage reaches to 1V. If we put these numbers into the equation, we get,

$$1 = 2 + [0.420 \ - 2]e^{-\frac{0,0068}{1000C}}$$

As we did before, the rest is just calculation.

$$1 = 2 + [0.420 \ - 2]e^{-\frac{0,0068}{1000C}}$$

$$-1 = [-1,58]e^{-\frac{0,0068}{1000C}}$$

$$0,632911 = e^{-\frac{0,0068}{1000C}}$$

$$-0,45742 = -\frac{0,0068}{1000C}$$

As a result, our C value is, 14.86uF, and it is close to the value that we found in simulation as well.

Part 2 - Studying Van der Waals (molecular) bonding for the inert gas crystal.

Question 1- Derive the analytical equation for the force F for the electrostatic potential energy as a function of the distance r

The Lennard-Jones potential is given by:

$$\mathrm{V(r)} = 4\varepsilon\left[\frac{\sigma^{12}}{r} - \frac{\sigma^{6}}{r}\right]$$

where **ε is the depth of the potential well** and **σ is the distance at which the potential is zero**.

The force can be obtained by taking the negative gradient of the potential:

$$F(r) = -\frac{dV(r)}{dr}$$

To calculate this derivative, we need to use the chain rule and the power rule:

$$F(r) = -d/dx\ [4\varepsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}]]$$

$$F(r) = -4\varepsilon\left[-\frac{12\sigma^{12}}{r^{13}} + \frac{6\sigma^{6}}{r^{7}}\right]$$

$$F(r) = \frac{48\varepsilon\sigma^{12}}{r^{13}} - \frac{24\varepsilon\sigma^{6}}{r^{7}}$$

Question 2- For the functions U(r) and F(r) investigate the extrema (minima and maxima) properties, and plot both functions.

First, let's consider the Lennard-Jones potential function:

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

To find the extrema of this function, we need to find its derivative which is equal to zero respect to r:

$$\frac{dV(r)}{dr} = -\frac{48\varepsilon\sigma^{12}}{r^{13}} + \frac{24\varepsilon\sigma^{6}}{r^{7}} = 0$$

Simplifying this expression, we get:

$$r_{\min} = 2^{\left(\frac{1}{6}\right)}\sigma$$

This represents the location of the minimum in the potential energy function, where the attractive forces between the atoms balance with the repulsive forces, leading to a stable equilibrium distance.

To find the extrema of the force function, we need to differentiate the force equation that we derived :

$$F(r) = \frac{48\varepsilon\sigma^{12}}{r^{13}} - \frac{24\varepsilon\sigma^{6}}{r^{7}}$$

$$\frac{dF(r)}{dr} = -\frac{624\varepsilon\sigma^{12}}{r^{14}} + \frac{168\varepsilon\sigma^{6}}{r^{8}}$$

Setting the derivative equal to zero and solving for r, we find:

$$r_{\max} = \left[\left(\frac{312\varepsilon\sigma^{12}}{84\varepsilon\sigma^{6}}\right)^{\frac{1}{6}}\right]\sigma$$

This represents the location of the maximum in the force function.

When we plot it on MATLAB

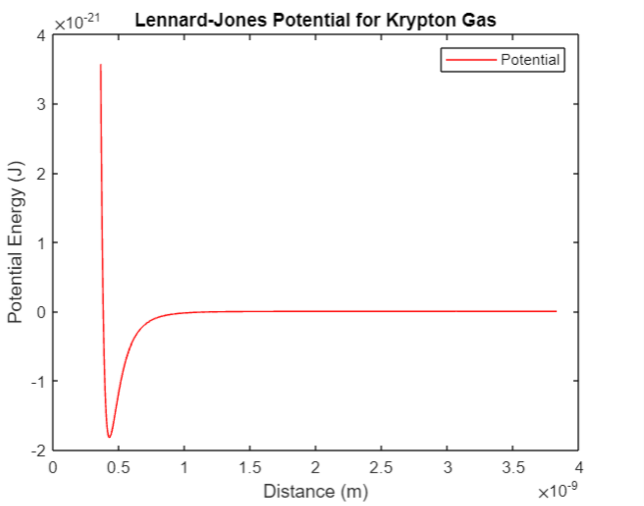

Figure 31 : The graph of Lennard-Jones potential

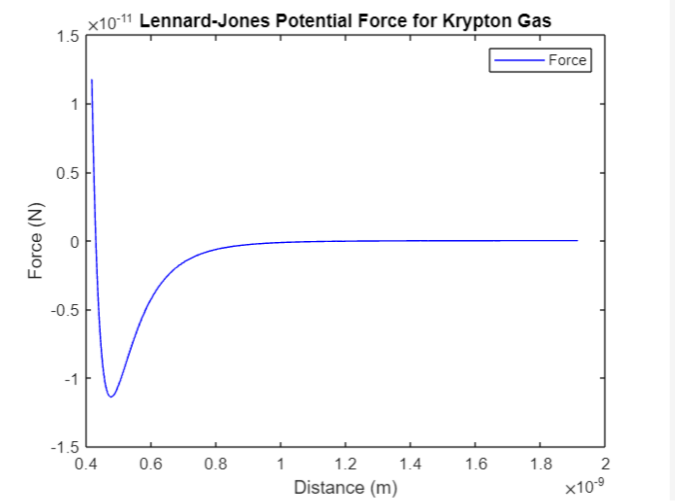

Figure 32 : The graph of Total force including Lennard-Jones and Coulombic contributions

Question 3- Find the equilibrium distant req for the Lennard-Jones potential.

The equilibrium distance, denoted as R_{eq} , is the distance at which the potential energy is at a minimum. In the case of the Lennard-Jones potential, the potential energy function is:

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

To find the minimum of this function, we can take its derivative with respect to r and set it equal to zero:

$$\frac{dV(r)}{dr} = -\frac{48\varepsilon\sigma^{12}}{r^{13}} + \frac{24\varepsilon\sigma^{6}}{r^{7}} = 0$$

Simplifying this expression, we can write:

$$\text{Req} = \sigma * \left(2^{\frac{1}{6}}\right)$$

Thus, the equilibrium distance for the Lennard-Jones potential is given by Req = σ*(2^(1/6)). This is the distance at which the attractive and repulsive forces balance out.

Question 4- Write the equation for the force F components F_x, F_y and F_z, in the Cartesian coordinates (considering the spherical symmetry of this force with respect to its radial measure r).

The force F(r) for the Lennard-Jones potential and the electrostatic potential energy can be expressed as:

$$F(r) = -\frac{dU(r)}{dr} - \frac{(e^2)}{4\pi\varepsilon 0 r^2}$$

U(r) is the Lennard-Jones potential energy function, k is the Coulomb constant, e is the charge on the particles, and r is the distance between them.

Since the potential has spherical symmetry, we can express the force components Fx, Fy, Fz in terms of the radial component F_r using the following equations:

$$Fx = Fr\ x \cos(\theta)\ x \sin(\varphi)$$

$$Fy = F_r x \sin(\theta)\ x \sin(\varphi)$$

$$Fz = Fr\ x \cos(\varphi)$$

Theta is the angle between the x-axis and the radial direction, and phi is the angle between the z-axis and the radial direction.

The radial component of the force F_r can be representedas:

$$Fr = -\frac{dU(r)}{dr} - \frac{(e^2)}{4\pi\varepsilon 0 r^2}$$

To find the expressions for the angular components of the force, we need to differentiate the expressions for Fx, Fy, and Fz with respect to theta and phi using the chain rule:

$$\frac{dFx}{d\theta} = Fr\ x\ (-\sin(\theta)\ x \sin(\varphi))$$

$$\frac{dFx}{d\varphi} = Fr\ x\ (\cos(\theta)\ x \cos(\varphi))$$

$$\frac{dFy}{d\theta} = Fr\ x\ (\cos(\theta)\ x \sin(\varphi))$$

$$\frac{dFy}{d\theta} = Fr\ x\ (\sin(\theta)\ x \cos(\varphi))$$

$$\frac{dFz}{d\theta} = 0$$

$$\frac{dFz}{d\varphi} = Fr\, x(-\sin(\varphi))$$

Therefore, the Cartesian components of the force can be expressed as:

$$Fx = \left(-\frac{dU(r)}{dr}\right) x \cos(\theta)\, x \sin(\varphi)$$

$$Fy = \left(-\frac{dU(r)}{dr}\right) x \sin(\theta)\, x \sin(\varphi)$$

$$Fz = \left(-\frac{dU(r)}{dr}\right) x \cos(\varphi)$$

Question 5- Find the Cartesian components of the gradient vector for U(r).

The gradient vector of a scalar function U(r) is a vector whose components are the partial derivatives of U. In Cartesian coordinates (x, y, z), the gradient vector is:

$$\nabla U(r) = \left(\frac{\partial U}{\partial x}\right) i + \left(\frac{\partial U}{\partial y}\right) j + \left(\frac{\partial U}{\partial z}\right) k$$

where i, j, and k are the unit vectors in the x, y, and z directions, respectively.

For the Lennard-Jones potential function, we have:

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

To find the Cartesian components of the gradient vector, we need to take the partial derivative of U with respect to each coordinate:

$$\frac{\partial U}{\partial x} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] * \left[\left(\frac{12\sigma^{12}}{r^{13}}\right) * \left(-\frac{x}{r}\right)\right]$$

$$\frac{\partial U}{\partial y} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] * \left[\left(\frac{12\sigma^{12}}{r^{13}}\right) * \left(-\frac{y}{r}\right)\right]$$

$$\frac{\partial U}{\partial z} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] * \left[\left(\frac{12\sigma^{12}}{r^{13}}\right) * \left(-\frac{z}{r}\right)\right]$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

Simplifying these expressions, we get:

$$\frac{\partial U}{\partial x} = -\frac{48\varepsilon\sigma^{12x}}{r^{14}} + \frac{24\varepsilon\sigma^{6x}}{r^{8}}$$

$$\frac{\partial U}{\partial y} = -\frac{48\varepsilon\sigma^{12y}}{r^{14}} + \frac{24\varepsilon\sigma^{6y}}{r^{8}}$$

$$\frac{\partial U}{\partial z} = -\frac{48\varepsilon\sigma^{12z}}{r^{14}} + \frac{24\varepsilon\sigma^{6z}}{r^{8}}$$

the Cartesian components of the gradient vector are:

$$\nabla U(r) = \left[-\frac{48\varepsilon\sigma^{12x}}{r^{14}} + \frac{24\varepsilon\sigma^{6x}}{r^{8}}\right]i + \left[-\frac{48\varepsilon\sigma^{12y}}{r^{14}} + \frac{24\varepsilon\sigma^{6y}}{r^{8}}\right]j + \left[-\frac{48\varepsilon\sigma^{12z}}{r^{14}} + \frac{24\varepsilon\sigma^{6z}}{r^{8}}\right]k$$

Question 6- Find the work W which is done by the Lennard-Jones force to transfer the electrical charge e from the initial position r = σ to infinity.

The work done by the Lennard-Jones force to transfer the electrical charge e from the initial position r = σ to infinity can be calculated using the following integral:

$$W = \int_{\sigma}^{\infty} F(r)dr$$

Lets look at the work and potential energy relation first:

$$W = U_{initial} - U_{final}$$

$$U_{initial} == 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Our initial point is r= σ so

$$U_{initial} == 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] = 0$$

Now let's look at the final potential

$$U_{final} == 4\varepsilon\left[\left(\frac{\sigma}{r+\Delta r}\right)^{12} - \left(\frac{\sigma}{r+\Delta r}\right)^{6}\right]$$

$$\Delta r = The\ dicrease\ on\ the\ radial\ distance\ of\ one\ of\ atoms\ because\ of\ ionization.$$

Now let's put the values inside the equation

$$W = U_{initial} - U_{final}$$

$$W = 0 - 4\varepsilon\left[\left(\frac{\sigma}{r+\Delta r}\right)^{12} - \left(\frac{\sigma}{r+\Delta r}\right)^{6}\right]$$

$$W = -4\varepsilon\left[\left(\frac{\sigma}{r+\Delta r}\right)^{12} - \left(\frac{\sigma}{r+\Delta r}\right)^{6}\right]$$

So we found that at r= σ our initial potential is zero, but our final potential will be negative because as you can see on the *Figure24* after our potential reaches to zero at σ point potential becomes negative that means our final potential is negative, but ***work*** is positive.

Part 3- Toy Model for the Resistance in the Cristal Lattice.

Electrons are not completely free to move in a conductor. The flow of electrons through a material undergoes many collisions, due to the fact that atoms are oscillating which hinders their motion. For this event, the mechanical correspondent is friction.

We can analyze this phenomena by using current definition and resistivity.

First we can define current as the amount of charge per unit time passes through a plane.

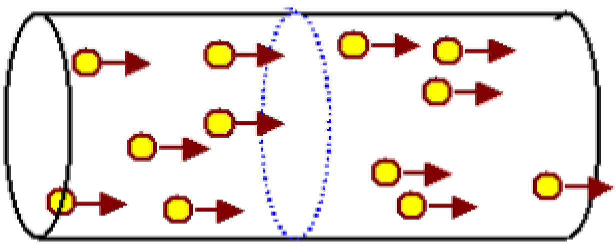

Figure 33 : The demonstration of movement of particles

The flow of charge through the cross-section of a conductor at a particular-point is described by current density, J which is vector quantity.

Definition,

$$i = \int \vec{J}.d\vec{A} \quad and\ i = J.A$$

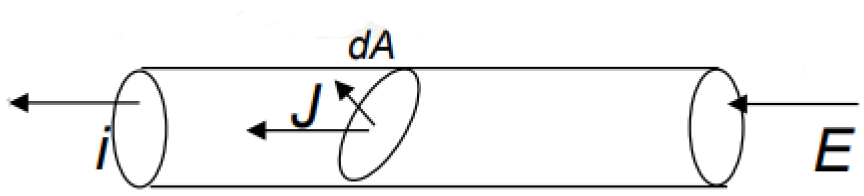

Figure 34 : Direction of current, current density and electric field

When a conductor has a current passing through it, the electrons move randomly, but they tend to drift with a drift speed V_d in the direction that of the applied electric field that causes the current.

Current density definition,

$$i = \frac{q}{t}$$

Total charge in length L with cross-section A

$$q = nALe$$

n is amount of charge and e is the magnitude of one electron charge,

Electrons move with drift speed so that time is

$$t = \frac{L}{V_d}$$

Then put them into $i = \frac{q}{t}$,

$$i = \frac{nALe}{\frac{L}{V_d}}$$

$$i = nAeV_d$$

$$V_d = \frac{i}{nAe}$$

We know that $\frac{i}{A} = J$

$$V_d = \frac{J}{ne}$$

$$(ne)\vec{V}_d = \vec{J}$$

As a result, Drift velocity and Current Density have the same direction.

About resistivity, we can use Ohm's Law and resistance formula as follows,

$$R = \rho\frac{L}{A} \quad and\ R = \frac{V}{i}$$

$$\rho\frac{L}{A} = \frac{V}{i}$$

$$\rho = \frac{V/L}{i/A}$$

$$\rho = \frac{E}{J}$$

So as a result we have defined resistivity in terms of electric field and current density.

When applying electric field on metal sample, the electrons amend their random motions slightly and drift with drift velocity due to the random collisions. If an electron of mass m is placed in an electric field, will experience an acceleration due to the force created by electric field,

$$a = \frac{F}{m}$$

We know $F = eE$ due to electric field,

$$a = \frac{eE}{m}$$

And We can define time τ as the average time between each collisions, between each collisions particles accelerates, and drift velocity changes during time as follows,

$$V_d = \tau\, a$$

$$V_d = \tau\frac{eE}{m}$$

From this equation $(ne)\vec{V}_d = \vec{J}$

$$(ne)\tau\frac{e\vec{E}}{m} = \vec{J}$$

If we arrange this,

$$\frac{\vec{E}}{\vec{J}} = \frac{m}{e^2 n\tau}$$

We know rate electric field to current density is resistivity from this equations $\rho = \frac{E}{J}$

$$\rho = \frac{m}{e^2 n\tau}$$

The part of $\frac{m}{e^2 n}$ is constant, so that we can make a comment on resistivity. Because of time dependence, resistivity is approximately equal to $\frac{1}{\tau}$.

$$\rho \approx \frac{1}{\tau}$$

From the given toy model to demonstrate the resistance in lattice, a particle moves in a corridor and in that corridor atoms of matter are oscillating. That oscillation depends on the temperature of matter. In lattice, when temperature is increasing, lattice ions and atoms vibrate more rigorously due to their thermal energy. Thermal energy and atomic motion are related to kinetic energy. With increasing in temperature kinetic energy increases and as a result oscillation increases, resulting in higher resistance.

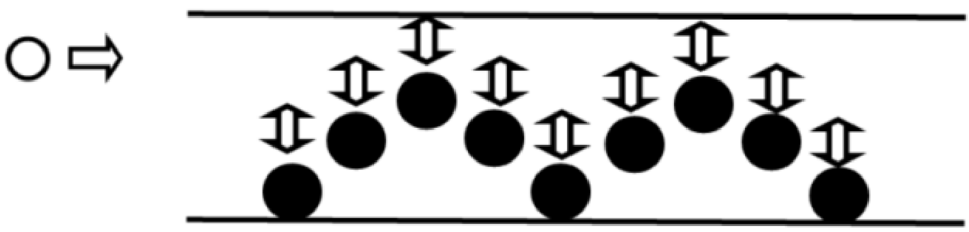

Figure 35 : Toy model for the resistance in the crystal lattice

As we defined resistivity with $\rho \approx \frac{1}{\tau}$, increases in temperature results in change of τ. The reason of change in τ is that when temperature increases, oscillating increases so that particle moving in lattice will hit the lattice ions with a greater number of collisions. And that hinders particle movement, and also because of gaining kinetic energy particle's drift velocity increases. So τ decreases. Thus resistivity increases.

And a final comment can be made as this, increasing temperature decreases τ. Consequently, the relation between resistivity and temperature in metals is linear,

$$\rho \approx T$$

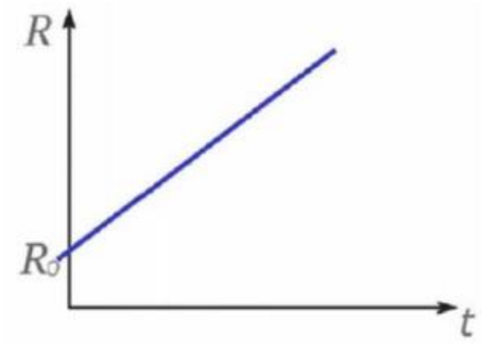

Figure 36 : The graph of dependence of resistance R vs temperature

The reason for the resistance R_0, after T=0 which is absolute zero, is that the lattice ions stop to oscillate. But they are still there, and a particle that moves into lattice may hit them, so this results in resistance because of the existence of lattice ions.

RESULTS AND DISCUSSION

Part 1 task 1 (for 1D) and task 2 (for 2D)

In this part of the project, we are asked to consider the electrostatic energy of an ionic lattice. In these lattices, we know that (+) signs represent Na atoms, (-) signs represent Cl atoms, and until they make a connection, these ions are electrically attracted to each another. When they come into touch, pushing them closer together attempting results in a powerful repulsive force. This information and $U = -a.\frac{q^2}{4\pi\varepsilon_0 \mathrm{R}_e}$ which is the equation of electrostatic potential energy were given to us.

For calculating the Madelung constant for 1D lattice, after choosing our reference point, according to the formula, we calculated the potential energy between Na-Na atoms and Na-Cl atoms. After making calculations, we collected them, and we rearranged in the form of summation symbol by paying attention to alternating harmonic series situation due to the signs of each term. After doing calculations, we get the Madelung constant as 2ln2 for 1D lattice.

For making numerical evaluation for 2D lattice, again we chose a Na ion as a reference point. After doing calculations which has some difference from calculating 1D lattice, we obtained Madelung constant as 1.613 by paying attention to the radiuses.

As we can see, the Madelung constants are different for 1D and 2D lattices. In a 1D lattice, ions are arranged in a single dimension so, electrostatic interactions occur between charges. For 2D lattice, electrostatic interactions happen both vertical and horizontal. So, two dimensional structures consist more interactions and this leads to have different Madelung constants.

Task 3a

For this part of the project, to generate different networks having 4, 16. 64, 128 and 256 nodes, we determined our r0 values as 10 ohms. To find the equivalent resistances of each network, our method is using Ohms Law. By using simulation tool, which is Proteus, after applying DC voltage, we obtained current value, so that we can calculate equivalent resistance. The reason why we apply the voltage form the middle of the circuit for each network is that we wanted to see how the equivalent resistance behaves as the number of nodes increases by giving the voltage from the same input.

Task 3b

For this part of the project, we studied in the lab to measure equivalent resistance for the 4 nodes and 16 nodes networks. As a test method, as we did in the simulation part for calculating equivalent resistance, we applied voltage using DC power supply device, then we obtained current value. For the network which has 4 nodes, we obtained equivalent resistance as we expected. We verified it. However, for the network which has 16 nodes, the equivalent resistance value was 7.69230 Ω. It is different from the Req, which was done in the simulation part, which is 7.315288. This difference is due to the tolerance of the resistance and due to the fact that cables that we used have resistance.

Task 4a

In this part of the project, we were asked to measure equivalent capacitance for the networks for, 4, 16, 64, 128 256 nodes by using simulation tool. The capacitance value we used is 10µF. As a test method for measuring equivalent capacitance, we designed a RC circuit to measure it. And we applied 100V DC source to observe the transient analysis. We obtained equivalent capacitance value by measuring how much time takes to reach from initial value to 63.2% of voltage value and this period of time is 1 time constant.

Task 4b

In this lab experiment, to measure equivalent capacitance for the networks of 4 and 16 nodes, we used function waveform generator to generate a square wave function, 0 to 2V and 10Hz and we observed the function of the voltage of capacitor network by using an oscilloscope.

For the first experiment, first we calibrated our probes to obtain better measurements. Then we connected signal generator to the circuit and put the probes ride after the resistance. Then we get signal function on the display of oscilloscope. We used the cursors in the track mode to measure first initial value and measure an arbitrary value. Next, we put the numbers, we get from cursor observation, into the formula. As we did for the first experiment, we applied the same steps for the second experiment and our results are as follows.

	Nodes	Signal type	Amplitude	Offset	Frequency	Resistance	Δt	V (0)	V(t)	Equivalent capacitance
Experiment 1	4	Square	2V	1V	10Hz	1kΩ	5.6ms	0.34V	1V	11.49 uF.
Experiment 2	16	Square	2V	1V	10Hz	1kΩ	6.8ms	0.42V	1V	14.86uF

CONCLUSIONS

In conclusion, the project focused on studying the electrostatic energy in ionic crystals, specifically NaCl salt crystal and inert gas crystals. The project was divided into three parts, each addressing different aspects of the topic. Part 1 examined the electrostatic energy of a 1D and 2D NaCl crystal lattice. The Madelung constant was found for the infinite 1D crystal, and the analytical series for the electrostatic potential energy was constructed. The van der Waals bonding in inert gas crystals was the topic of Part 2. We introduced the Lennard-Jones potential and looked at some of its features, including force and equilibrium distance. Part 3 presented a toy model that represented the resistance in a crystal lattice. The model illustrated the interaction between moving electrons and oscillating ions in a metal lattice, which contributes to the electrical resistance. Throughout the project, both analytical and numerical approaches were utilized. Simulation tools were employed to evaluate equivalent resistance and capacitance in resistor and capacitor networks.

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