

TNL

THz Spectroscopy Simulator (TNL-TS Simulator) Tutorial

Material Characterization simulation Software



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1stFeb,2021

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1.1 Getting Started

To use the TNL THz Spectroscopy simulator (TNL-TS simulator) user needs to get the license for this. Once they get the license for the same, they can verify it by opening the TNL-Framework. At framework user will see a tick mark on the side of the name Spectroscopy in green color which confirms the license for same as represented in figure 1 below. But if a cross mark in red color is present then user might not using valid license (in this case user needs to contact TNL Pvt. Ltd.). For more information user needs to go through the License Manual.

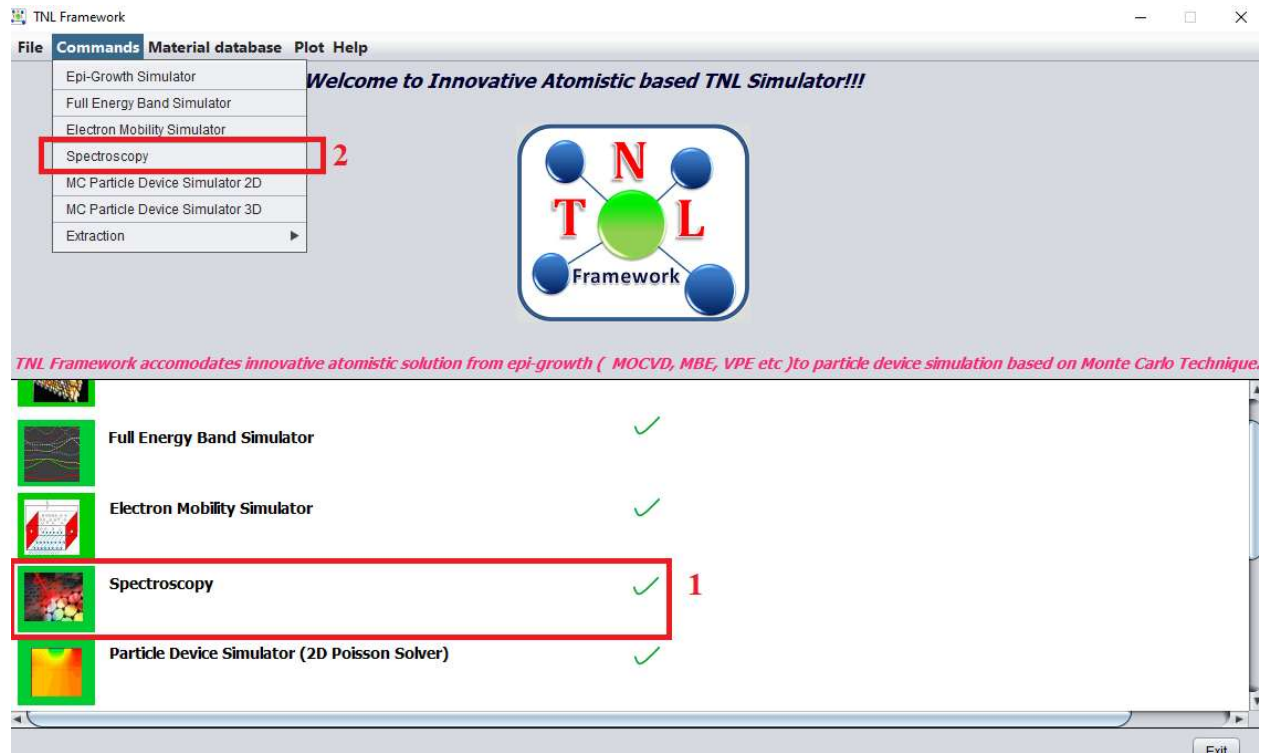


Figure 1 : TNL-Framework

There are two ways to open the TNL-TS SIMULATOR from the Framework shown in figure1. Those ways are shown in red rectangular boxes (box1 and box2).

1. This box1 contains TS Simulator's icon and name. By a single click on icon or name user gets access to use the simulator
2. This box2 contains sub menu named as Spectroscopy. By clicking on the menu Command user will get several sub-menus containing the names of all simulators of TNL family. By a single click on name user gets access to use the simulator.

Using any of the above two methods user will be directed to the TNL-TSSimulator window frame THz Spectroscopy Simulator as shown in figure2.

1.2 TNL-TS SIMULATOR window frame

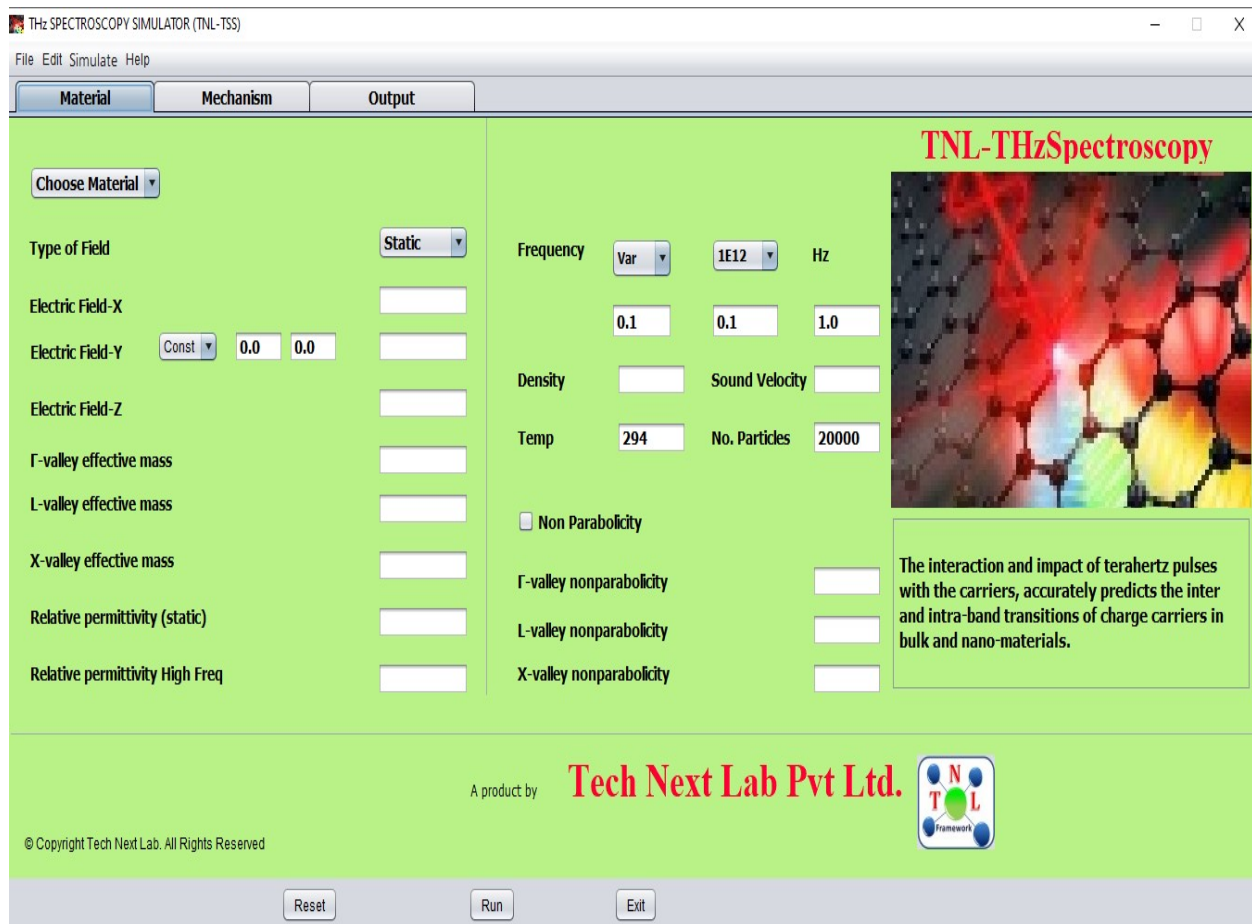


Figure 2: THz Spectroscopy Simulator window frame.

TNL-TS SIMULATOR window frame in figure 2 contains several tabs named as:

1. Material
2. Mechanism
3. Output

1.2.1 Material tab

Here several drop boxes and text fields are given containing input information regarding material, electric field, frequency, mass, permittivity, density, velocity, temperature, particles and non-parabolicity factor. We will discuss it one by one.

1.2.1.1 Choose material

- Clicking on the **Choose Material** dropbox a menu containing several materials names will be shown like shown in figure 3.
- Various semiconductor materials database is available in the simulator, e.g. Si, Ge, GaAs, InP, AlAs, InAs, GaP, GaN, InN, ZnO etc.
- Users may choose any of the material as per requirement.
- One more option available here for defining user defined ternary material by choosing User-Defined option from here. When user chooses this option a new pop-up window will open as shown in figure 4(a).

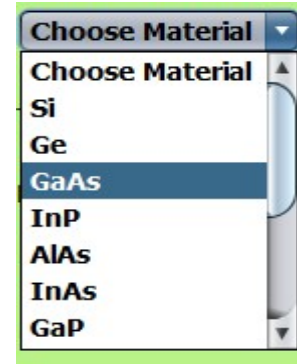


Fig 3: Choose material

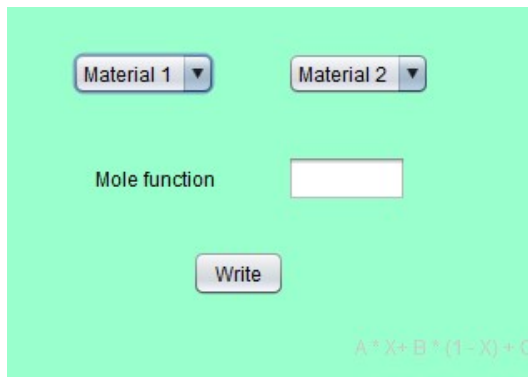


Figure 4(a)

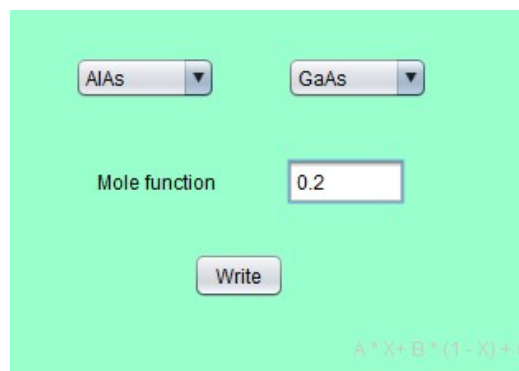


Figure 4(b)

The new pop-up window has options of material 1, material 2, mole function and write button. For example if user wants to do simulations for ternary material like $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ ($\text{Al}_x\text{Ga}_{1-x}\text{As}$). So they need to choose AlAs and GaAs from Material1 and Material2 options respectively. Then they need to give mole fraction value required for his defined material, 0.2 in this example. Now they have to click the “Write” button at the bottom. Users will get back to the material tab of the simulator’s frame. Here now you will see besides the choose material (User-Defined) drop-box a text-field and a “Load” button is visible. When you will click on it the text-field will show your defined material ($\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$).

The simulator is connected to the inbuilt database of the most of the semiconductor materials given here and also it will interpolate the values of the user-defined materials. So by choosing any of the materials simulator will provides those default data from database as shown in figure 5.



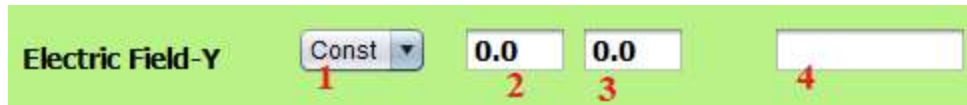
Figure 5: Default values of Ge.

While you choose a material the parameters like relative mass, permittivity, density and sound velocity of that material will be loaded automatically. All these fields values are editable, so user can input their value as per the requirement.

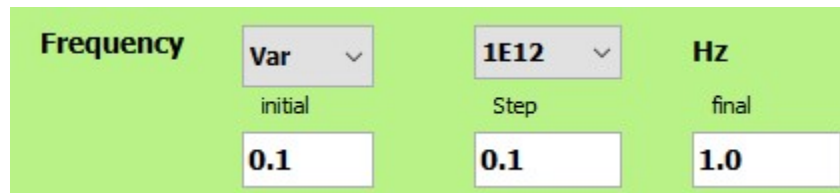
1.2.1.2 Biasing

After choosing the material, the biasing value is required to ramp the THz pulses. With the present formulation of the simulator, user needs to input the two parameters of the biasing. First is peak electric field value and second are frequency values to ramp the THz pulse. The biasing involves three values called initial, step and final. Initial value is that point at which point simulation will start first. Final value is the point upto which value the simulation will continue. Between these initial and final values, the step which means biasing will ramp from initial and final value with those step values and those are the intermediate simulation points.

Suppose user gives initial value 0, step value 0.1 and final value 1. Then the simulation will first start at the 0 then it will proceed to 0.1, 0.2, 0.3, ..., upto final value 1. During the simulation all respective output results will be saved at these step points (we will talk about it later in this tutorial). In this version we have provided vulnerability to ramp only the Frequency. In next version, users will find flexibilities to provide varying electric field also with the frequencies.

A: Electric-Field**Figure 6:** Electric- Field value

User can enter the values in the textbox fields in any direction of the the sample i.e. x, y, and z through Electric Field-X, Electric Field-Y, and Electric Field-Z. With the Electric Field-Y four options are given numbered 1 to 4 as shown in above figure. 1 is showing dropbox that contains Const (constant) as it's option in this version of simulator (*in next version we will open option for variable, so user can ramp electric field in y direction). 2,3 and 4 options are showing initial, step and final value to be inputted to ramp the electric field. In this version field 2 and 3 are kept fixed at 0kV/cm. So user needs to give the peak electric field value at field 4 as above. The unit of all electric field in x, y and z direction will be taken as kV/cm. Suppose you give value 10 in the field4 the simulator will take it as 10kV/cm.

B: Frequency**Figure 7:** Frequency value

Similarly user needs to provide the frequency values to biasing. They can give either variable or a constant frequency by choosing options Var/Const in first dropbox. The second dropbox contains value 1E12 Hz as we are performing simulation on sample at THz frequency. There are three fields for initial, step and final values user may provide require value similarly as per their THz experiments. If Const is chosen you need to give equal value to all these fields.

Note: *Please give your initial value equal to or greater than 0.1 for frequency.*

1.2.1.3 No. of Particles

Users may input the number of particles to initialize the simulation. These particles can be distributed over the three valleys described in section 1.2.2.2. The number of particles is contributing to the energy level calculations and further use in calculating various scattering rates. By-default 20000 particles are taken in this field; user may change this value as per their requirement. There are tradeoff between number of particles used and simulation time. More

number of particles means more accurate results. More number of particles leads to more complex and lengthy computation and can increase the simulation time.

1.2.1.4 Temp

This field represents to the temperature; at which user needs to run the simulation on the sample and they can analyze the effect of the temperature dependence of on the output results. The temperature value has been taken in unit of kelvin (K) in simulator.

1.2.1.5 Non-Parabolicity



Non Parabolicity

Γ -valley nonparabolicity

L-valley nonparabolicity

X-valley nonparabolicity

Figure 8: Non Parabolicity

Under material tab there is a check-box named Non Parabolicity, by default it is unchecked means simulator is not considering non-parabolicity effect of the energy bands. User may select it by clicking the check box, the respective values of nonparabolicity values of energy bands at various valleys of selected material will be loaded and will be shown in the fields given below named gamma, L and X valley nonparabolicity from the database.

1.2.2 Mechanism tab

Mechanism tab contains various scattering mechanisms options and various material properties require initializing the simulation. TNL-TS simulator contains most of scattering mechanisms e.g. lattice scattering, acoustic scattering, defect scattering, carrier-carrier scattering and other scatterings.

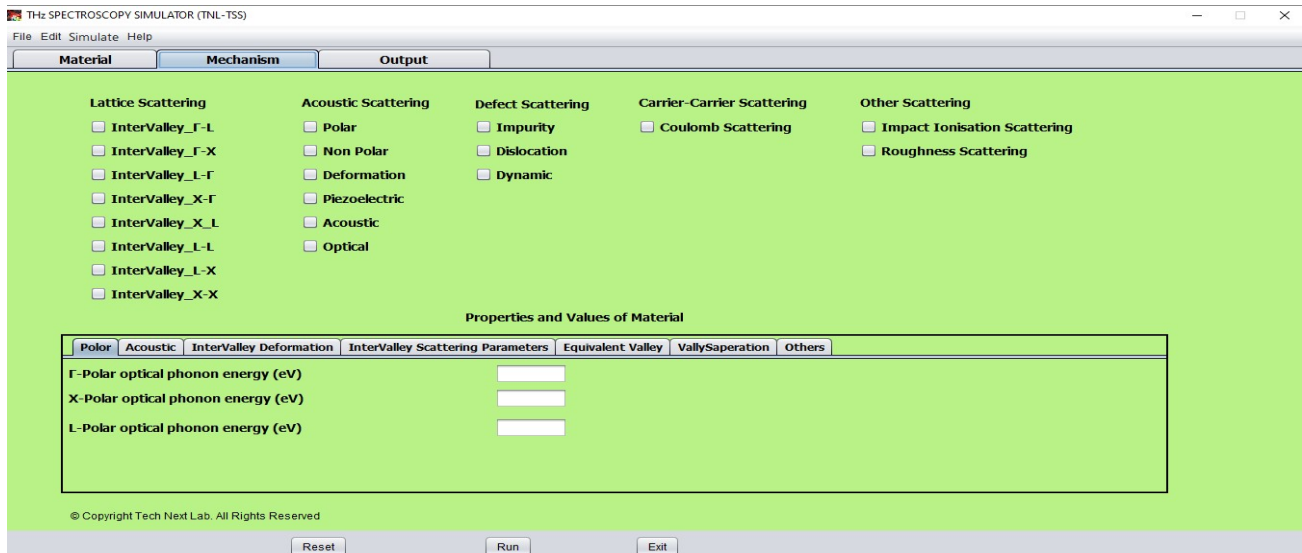


Figure 9: Mechanism frame

1.2.2.1 Scattering Mechanisms

A: Lattice scattering

It contains all intervalley scattering mechanisms

- i. Gamma to L (InterValley_Γ-L)
- ii. Gamma to X (InterValley_Γ-X)
- iii. L to Gamma (InterValley_L-Γ)
- iv. L to X (InterValley_L-X)
- v. L to L (InterValley_L-L)
- vi. X to Gamma (InterValley_X-Γ)
- vii. X to L (InterValley_X-L)
- viii. X to X (InterValley_X-X)

B: Acoustic Scattering

- i. Polar
- ii. Non-Polar
- iii. Deformation
- iv. Piezoelectric
- v. Acoustic
- vi. Optical

C: Defect Scattering

- i. Impurity
- ii. Dislocation
- iii. Dynamic

D: Carrier-carrier Scattering

- i. Coulomb

E: Other Scattering

- i. Impact Ionization
- ii. Roughness

1.2.2.2 Properties and values of material

The image shows a software interface window titled "Properties and Values of Material". It features a tabbed interface with the following tabs: "Polar", "Acoustic", "InterValley Deformation", "InterValley Scattering Parameters", "Equivalent Valley", "VallySaperation", and "Others". The "Polar" tab is currently active, displaying three input fields for the following parameters: "Gamma-Polar optical phonon energy (eV)", "X-Polar optical phonon energy (eV)", and "L-Polar optical phonon energy (eV)". Each input field is represented by a small white rectangular box.

Figure 10: Various tab for energies value of parameters of material.

These are the important semiconductor properties used during simulation involving in scattering rates and other complex parameters calculations during carrier motion. These values are for the lattice structural, thermal, elastic, lattice dynamics, electronic energy-band structural, optical and carrier transport properties of semiconducting materials. These values play an important role in THz simulation, so user need to be careful and decisive about these parameter values.

By-default simulator loads values of the associated material of his choice as discussed in material section. (these values have been taken from various reputed literature and calibrated with experiments). However, users have flexibility to edit these values from their perspective which will be reflected in the change in output results. The parameters are shown as:

1. Polar

This tab contains polar optical phonon energies of Γ , L and X valley in eV of material.

2. Acoustic

This tab contains acoustic deformation potential of Γ , L and X valley in eV of material.

3. Intervalley Deformation

A deformation potential is a quantity proportional to a matrix element of an operator belonging to a crystal deformation between a final and initial electron state. It has the units of eV.

4. Intervalley Scattering

This tab contains phonon energy between the two valley of Γ , L and X valley in eV of material.

5. Equivalent Valley

This tab contains no. of equivalent valley for each of the Γ , L and X valleys in same Brillouin zone.

6. Valley Separation

The tab contains fields where user need to give the value corresponding to energy difference between the lower points of the two valleys. The simulator is taking gamma (Γ) valley as a reference point. So, it is required to consider the separation of X and L valley with respect to Γ valley. This separation may be a positive or a negative value depending upon the exact positions of the satellite valley with the reference Γ valley with energy value zero. The unit of this separation is in eV.

7. Others

This tab has several fields some of which are related to the scattering, some are with the doping of material and initial position of particles used in simulation.

- i. **Alloy disorder:** This is the scattering rate user need to provide when he will select the dynamic scattering from the column of defect scattering in this mechanism window.
- ii. **Line dislocation:** This is the scattering rate user need to provide when he will select the dislocation scattering from the column of defect scattering in this mechanism window.
- iii. **Ionized impurity:** This is the concentration of the impurity present in the sample material which needs to be provided when user will select the Impurity scattering from the column of defect scattering in this mechanism window.
- iv. **Piezoelectric coefficient:** This is the coefficient rate value need to provide when user will select the piezoelectric scattering from the column of acoustic scattering in this mechanism window. This coefficient is related to the volume change when a piezoelectric material is subject to the electric field or polarization on applied stress.
- v. **Doping density:** This is the doping concentration of the sample.
- vi. **Particle distribution in each valley:**

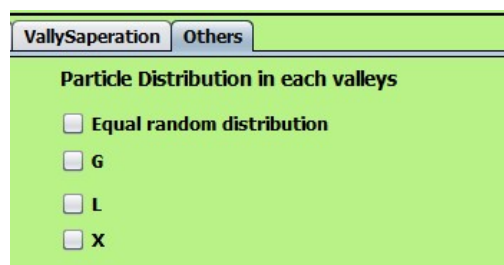


Figure11: Particle distribution

Simulator provides flexibility to the user to choose no. of particles for initial distribution as described in section 1.2.1.3 to the three valleys as shown in figure 11. There are four options given to do distribution like equal random distribution, Γ , L and X. If user selects equal random distribution the no. of particles initialized will be almost equally distributed with help of random technique in-built in the simulator. At this time all other three check-box will hide. If user do not select equal random distribution other three option will be available (Γ , L and X) and can choose any of these, then all particles will be initialized only in that particular valley.

In steady state condition zero field most of the particles try to occupy the lowest energy level follow the Aufbau principle. Algorithm of the simulator is designed in such a way that irrespective of the initial distribution of particles by users, particle will follow Aufbau principle and after a short time interval most of the particles residing at higher energy states will be depopulated to lowest lying energy state under steady state conditions.

1.2.3 Output Tab

This tab consists of two columns named Input script i.e. the material and its parameters and scattering models chosen and the output running script.

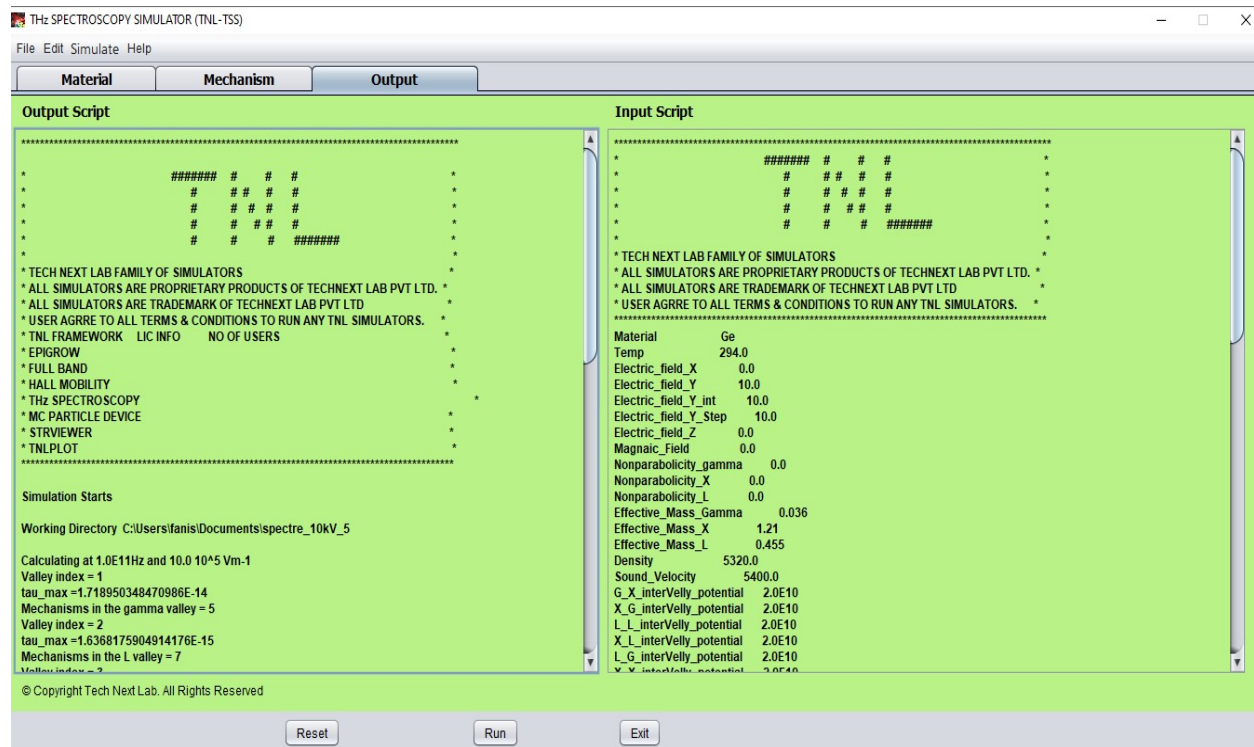


Figure 12: Output tab

1. Input script

This section shows all the input material parameter values and scattering mechanism information taken in Material and Mechanism section by the user, before clicking the “Run” button. User can check here all the input values before simulation start at this section.

2. Output script

This column will show the simulation points and it's some value of each bias point. As the simulation starts it will show the directory where all the simulation results will be saved with the line named working directory. After this some value of each bias point will be shown with the line named calculating at x Hz and y V/m. At the end of last bias point it will write a line Simulation Completed which notify user the successful completion of whole simulation after that they can see the results going to the working directory of respective simulation.

1.2.4Other

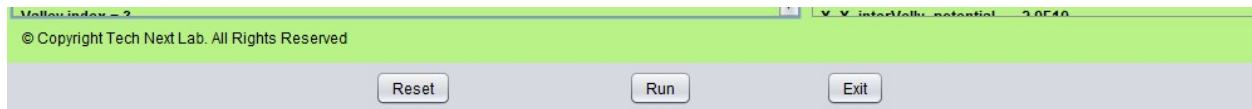


Figure 12: Other buttons

1. Run Button

To start the simulation user needs to press this Run button shown in figure 12. As user will press this button a pop window will open named save as shown in figure 13. By-default the selected directory will be ‘Documents’ of user computer, user can select any other directory of his computer. Then he needs to give the name of his simulation folder in the ‘File Name’ space and then press the ‘Save’ button. Thus, the working directory will be selected and all simulation will be saved in that folder.

2. Reset Button

After pressing this button all the fields in all tabs will get reset.

3. Exit Button

This button is used to exit the simulation and simulator will get close.

2. Hands-On

Now we will show a hands-on demonstration of the TNL-TS simulator using knowledge of description written in above sections. The simulation of Ge material at 181kV/cm of externally applied peak electric field value at room temperature using 20000 particles equally distributed in three valleys at a time with frequency ramp from 0.1 THz to 1THz and specific scattering parameters. Use following steps:

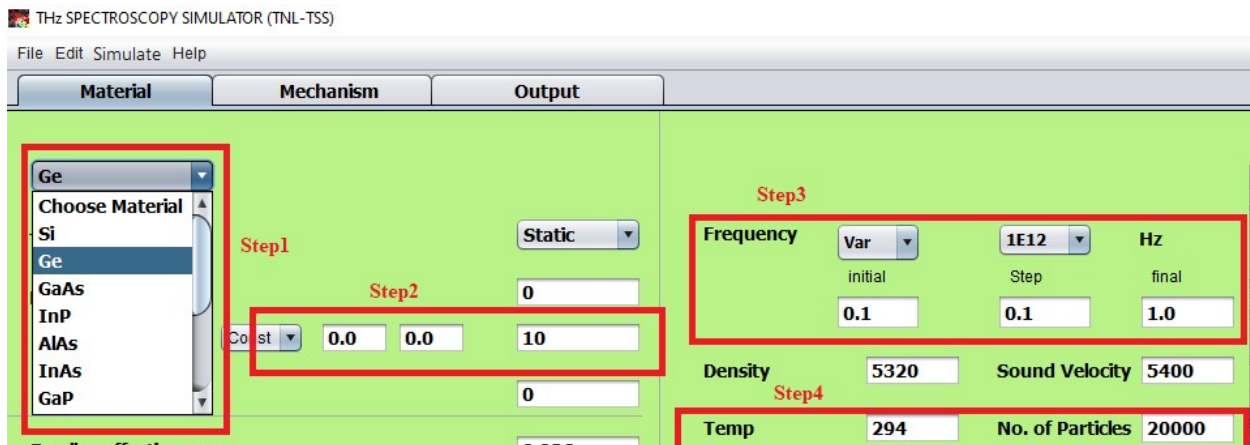


Figure 13:

Step 1: In material tab select Ge from the Choose material options. After clicking on Ge there some of the parameter will be loaded as shown in above figure 13 ins step1 red box.



Figure 14: Material tab showing five steps in red and black boxes.

Step 2: In this step as shown in Step 2 box in figure 14.

- i. Select Const.
- ii. Write 0 in Electric Field-X and Electric Field-Z.
- iii. Write 181 in final box of Electric Field-Y.

Step 3: In this step define the frequency value and type input in the bias as shown in Step 3 box shown in figure 14.

- i. Select Var.
 - ii. Select 1E12 Hz.
 - iii. Write 0.1 in initial, 0.1 in step and 1 in final fields.
- It will vary your frequency from 0.1 to 1 THz with step of 0.1THz.

Step 4:

- i. Write 294 in Temp field.
- ii. Write 20000 in No. of Particles field.

Step 5: Define non-parabolicity value of material. Here we have not chosen in this example. But if you want to include non-parabolicity perform following steps

- i. Select Non-Parabolicity check box.
- ii. Write non-parabolicity factor value of each valley.

Step 6: Click on Mechanism tab. Mechanism will open as shown in figure 15.

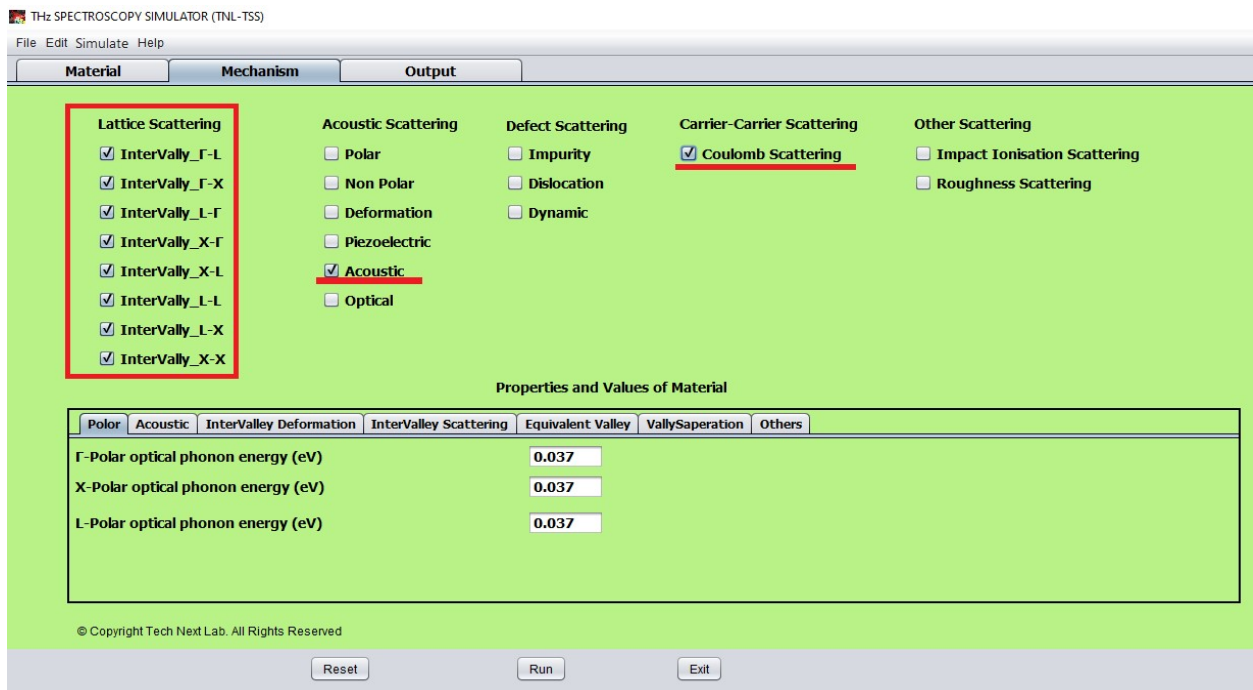


Figure 15: Mechanism tab with selected scattering mechanism (Lattice, Acoustic and Coulomb).

Step 7: As we need to select at least one scattering mechanism for successful simulation, here we have selected intervalley, acoustic and coulomb scatterings mechanisms.

Step 8: Now go to the Properties and Values of material. As we have selected the Ge material in Step1 all of the necessary values here have been pre filled. But if we need to do some modification perform following steps either skip to step 15.

Step 9: Click on Polar tab and write the required value in each field.

Step 10: Click on Acoustic tab and write the required value in each field.

Step 11: Click on Intervalley Deformation tab and write the required value in each field.

Step 12: Click on Intervalley Scattering tab and write the required value in each field.

Step 13: Click on Equivalent Valley tab and write the required value in each field.

Step 14: Click on Valley Separation and write the required value in each field.

Step 15: Click on Other tab.

Polar	Acoustic	InterValley Deformation	InterValley Scattering	Equivalent Valley	VallySaperation	Others
Alloy Disorder Scattering				<input type="text" value="0"/>	Particle Distribution in each valleys	
Line Dislocation				<input type="text" value="0"/>	<input checked="" type="checkbox"/> Equal random distribution	
Ionized impurity				<input type="text" value="0"/>		
Piezoelectric Coefficient				<input type="text" value="0"/>		
Doping density				<input type="text" value="9E22"/>		

Figure 16:

- i. As we have not selected any of the defect scatterings and piezoelectric scattering so we will not give any value to first four fields (leave as it is).
- ii. Give doping density value 9E22 for doping of ($9 \cdot 10^{22}$ per cm^3) to the sample material chosen.
- iii. Now select Equal random distribution check box.

Step 16: Click on Output tab.

Step 17: Click on Run button. A Save pop-up window opened as shown in figure 17.

Step 18: In save window default directory is ‘Documents’. Go to field named File name and write name of your file name (TNL-TS Simulator hand on for this example) to create a folder in the ‘Documents’ path of your system.

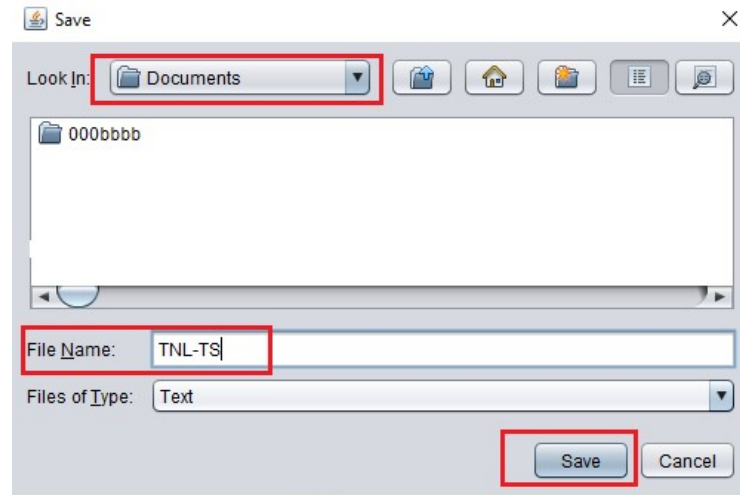


Figure 17: Save window.

Step 18: Now click Save button. With this step will start and you can see the input and output in the Input Script and Output Script of the Output tab. Output script column shows the working directory “C:\Users\...\Documents\TNL-TS”. It also shows “Calculating at 1.0E11Hz and 181 10⁵Vm⁻¹” as we have given the starting frequency 0.1*10¹² Hz.

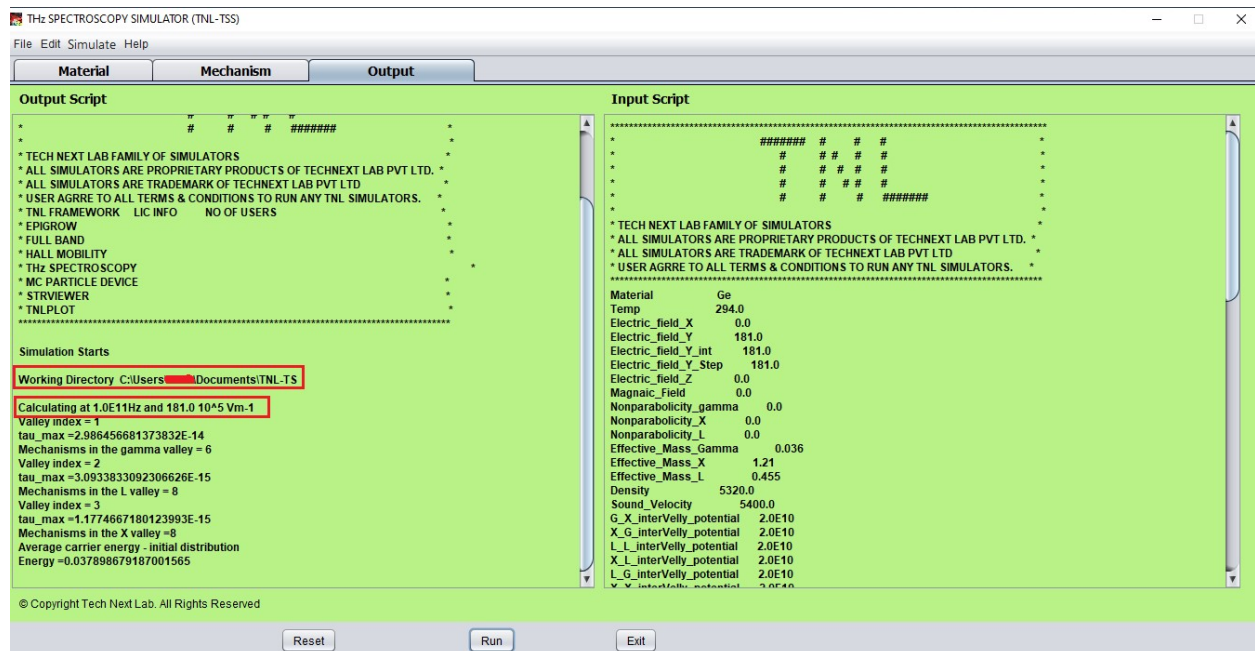


Figure 18: Output window

Step 19: Simulation will go for 0.1, 0.2, ... ,1.0 THz frequency and at last Simulation Completed message will be displayed in Output Script.

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Step 20: After the completion of simulation, go to the directory you selected there is a folder named TNL-TS.

Step 21: Open this folder, there are several folder and text file as shown in figure

Name	Date modified	Type	Size
Freq_1.0E11	2/6/2021 6:13 PM	File folder	
Freq_1.0E12	2/6/2021 6:40 PM	File folder	
Freq_2.0E11	2/6/2021 6:16 PM	File folder	
Freq_3.0E11	2/6/2021 6:18 PM	File folder	
Freq_4.0E11	2/6/2021 6:21 PM	File folder	
Freq_5.0E11	2/6/2021 6:24 PM	File folder	
Freq_6.0E11	2/6/2021 6:27 PM	File folder	
Freq_7.0E11	2/6/2021 6:30 PM	File folder	
Freq_8.0E11	2/6/2021 6:33 PM	File folder	
Freq_9.0E11	2/6/2021 6:37 PM	File folder	
plot	2/6/2021 6:13 PM	File folder	
TNL-TS	2/6/2021 6:13 PM	Text Document	5 KB

Figure 19: Output folder.

- i. In this folder you get folder at each frequency bias point named Freq_1.0E11 etc. , plot and a text file named TNL_TS. Each bias point folder contains a folder named E_field_181.0kV. Open this field folder which contains various file related to the simulation.
- ii. So, we will get all the information of th Ge material our applied electric field in y-direction at each frequency point.
- iii. Open any of these folders we will get files related to the scatterings selected, like acoustic, coulomb and intervalley for each valley. These contain scattering rates with respect to the energy levels.
- iv. Valley occupation files containing valley population at any time instant at that particular frequency.
- v. L, X and Gamma renormalized table value.
- vi. Velocity time averages in x, y and z direction.
- vii. Electric field vs time file at that particular frequency.
- viii. In plot folder the outputs data of simulation are
 - 1) current_density_vs_time,
 - 2) velocity_vs_time,
 - 3) Frequency_vs_Absorption,
 - 4) Frequency_vs_Conductivity,
 - 5) L-plot,
 - 6) X-plot and
 - 7) Gamma-plot.
- ix. We can plot these results on **TNL-PLOT** by importing the data file.
- x. The text file contains all the input parameter given to the simulator.