

**TNL**

**TNL-EMS**  
**Electron Mobility Simulator**  
**User Manual**  
**Material Characterization simulation Software**

**Tech Next Lab (P) Ltd**

Building No. #417/22/A, NiwazGanj,  
Near Napier Road Park, Lucknow - 226 003, (U.P.), India,

Tel: **(+91) 522 404 1565,**

Web: [www.technextlab.com](http://www.technextlab.com)

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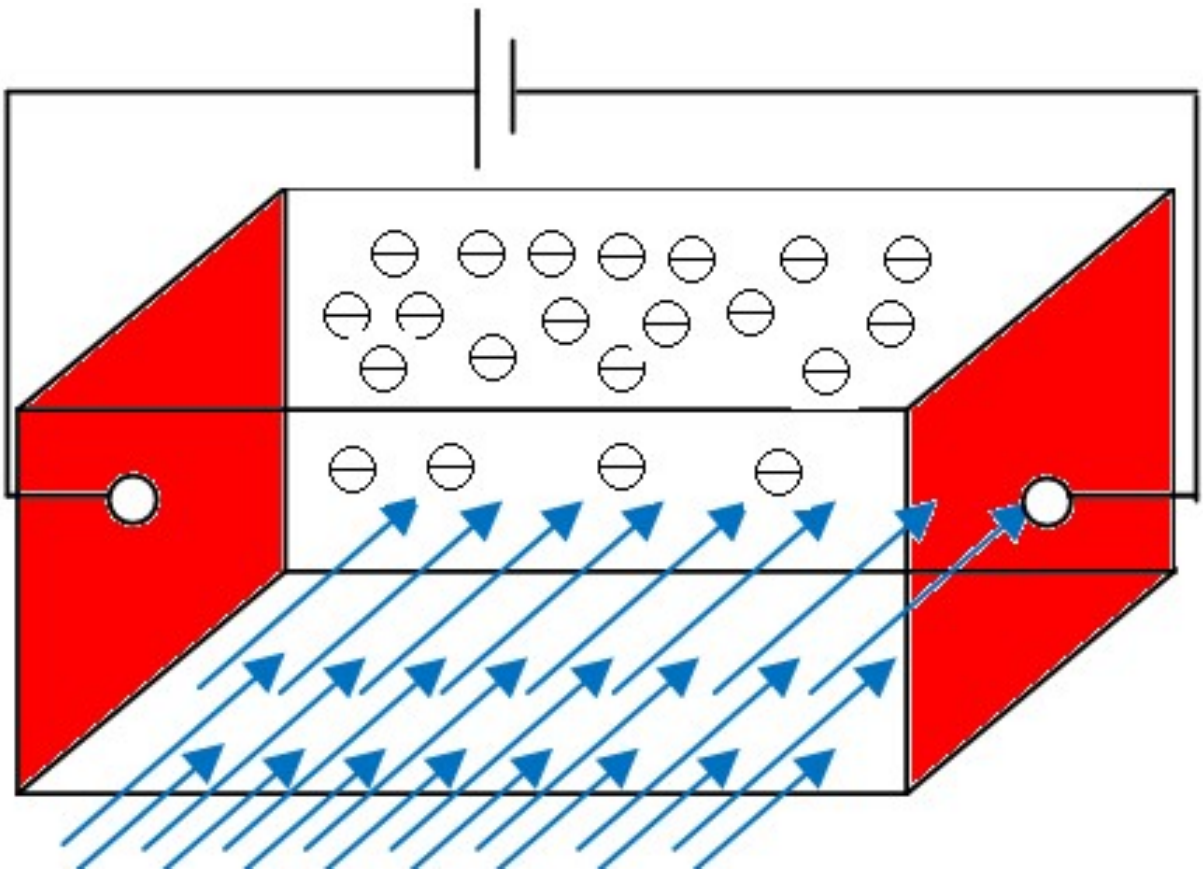
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# CHAPTER 1

## INTRODUCTION



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### **1.1 Electron Mobility Simulator (TNL-EMS) Overview**

Electron Mobility Simulator (TNL-EMS) is a powerful tool to simulate carrier transport on a full energy band or on a few valleys under the influence of an external electric field to accurately predict the carrier's mobility. The microscopic effect of the motion of individual particles in the presence of the forces acting on them due to the external fields and the internal fields generated from the crystal lattice and other charges in the system have been included in the TNL-EM simulator. In solids, such as semiconductors and metals, transport is known to be dominated by random scattering events due to impurities, lattice vibrations, etc., which randomize the momentum and energy of charge particles in time. Hence, stochastic techniques to model these random scattering events are particularly useful in describing electronic transport in semiconductors, in particular the Monte Carlo method. The Monte Carlo method inbuilt in TNL-EM simulator for solution of Boltzmann transport equation including non-linear scattering mechanisms provides flexibility to initialize the carriers over a full energy band or on a few valleys to analyze the transport of carriers to simulate the ensemble velocity of charge carriers under external electrical or electro-magnetic forces. The algorithms of TNL-EM simulator include the Monte Carlo technique which improves the "state-of-the-art" treatment of high-energy carrier dynamics. The detailed understanding of the capabilities of TNL-EM simulator is mentioned in the remaining chapters.

### **1.2 Need of Electron Mobility Simulator**

The following trends in the semiconductor industry are occurring concurrently with rapid changes in the applications of various semiconductor materials. The competitiveness among many semiconductor manufacturers is shifting from an emphasis on technology and fabrication to a much greater emphasis on product design, architecture, algorithm, and software; i.e., shifting from technology oriented R&D to product-oriented R&D in which computers, modeling, and simulation become increasingly crucial for marketplace success. In the marketplace there is no commercial software tool available for simulation of semiconductor material characterization such as carrier mobility and Hall mobility under the influence of an electromagnetic field. Researchers can do experimental Hall measurements which ultimately provide the Hall mobility

values of particular sample without giving any information about the insight physical mechanisms occurring due to impact of electromagnetic field.

The drift-diffusion and hydrodynamic models are the continuum methods of describing electronic transport in semiconductors, specifically which are derived from moments of the semi-classical Boltzmann Transport Equation (BTE). As approximations to the BTE, it is expected that at some limit, such approaches become inaccurate, or fail completely. Indeed, one can envision that, as physical dimensions are scaled upto 90nm and below, at some level a continuum description of current breaks down and the granular nature of the individual charge particles constituting the charge density in the active device region become important.

TNL-EM simulator is purely physics-based mobility simulator. A brief overview of TNL-EM simulator is provided here to serve as a high-level orientation. It can accurately predicts the carrier mobility characteristics with all other carrier transport properties including different scattering mechanisms on full or few valleys on the electronic band structure that are associated with specified physical semiconductor material sample under the influence of external electric field. The atomistic physic based simulation provides three major advantages:

- it is predictive,
- it provides real insight,
- it captures theoretical knowledge in a way that makes this knowledge available to non-experts.

Physically-based simulation is different from empirical modeling. TNL-EM simulator provides atomistic physics based simulation capabilities which can be used to accurately demonstrate the experiments as a source of data. Physically-based simulation has become very important from technology developments point of views for two reasons. First, it is almost always much quicker and cheaper than performing hit & trail experiments. Second, it provides information that is difficult or impossible to measure.

In the TNL-EM simulator, the solution of seven dimensional Boltzmann transport equation (BTE) is carried out under the influence of external electric field including various non-linear scattering mechanisms. The simulator help in extracting the various information associated with the carriers transport as output of simulation e.g. position, momentum, energy, drift velocity, mobility and other carrier transport properties.

### 1.3 TNL-EM simulator Features

- Graphical User Interface (GUI) based simulator i.e. no need for coding & scripting,
- User Friendly with Windows based application with full capabilities
- Boltzmann transport equation (BTE) solution without any initial assumptions
- Ensemble Monte Carlo Technique used for BTE solution
- Include various non-linear scattering mechanisms to calibrate the experiments
- Fermi Golden Rule for momentum & energy conservation
- Modeled beyond the effective-mass approximation on the full electronic band structure obtained from TNL-FB simulator
- The electron-phonon, electron-impurity, and electron-electron scattering rates included in a way consistent with the full band structure of the solid
- Accounting for density-of-states and matrix-element effects more accurately
- The carrier transport on the full energy band under influence of electromagnetic forces
- Users may trace all the carrier electronic transport properties associated with each single electron
- Bunches of examples inbuilt
- User defined materials can be accommodated easily
- Accurate up to a single particle level

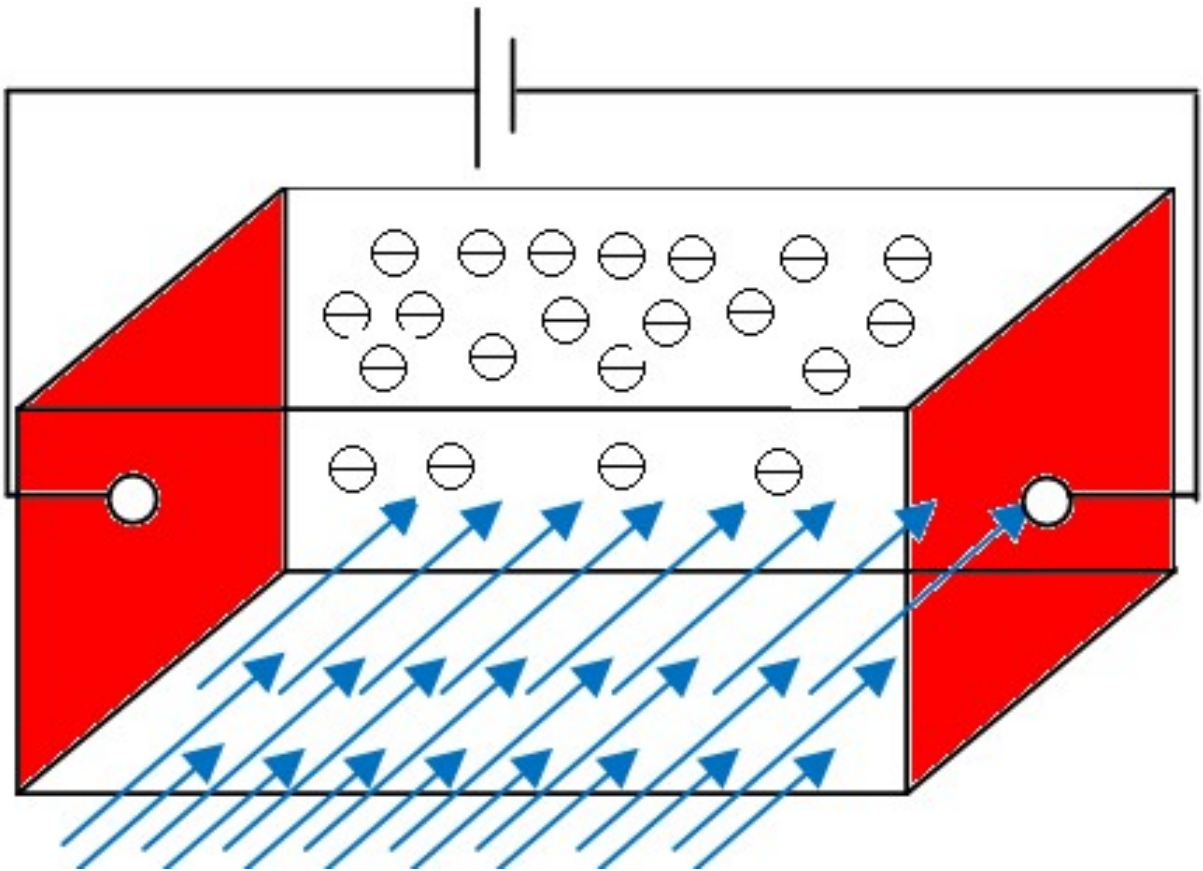


#### **1.4 Benefits can be realized from TNL-EM simulator**

- User Friendly
- GUI based simulator
- Fast and efficient algorithms
- Users may check all the run outputs during simulation running environment
- Purely atomistic physics based modeling capabilities
- Elemental, binary and ternary compound semiconductors database available
- Users can input electric & magnetic field
- Carrier transport on Full Electronic Energy Band or on few valleys
- Extraction of velocity of carriers under external forces
- Input database available for initial parameters
- Transport on parabolic & nonparabolic energy bands
- Different scattering mechanisms can be chosen for calibration of experimental results
- Ability to deal with different cubic, zincblende (Zb) & wurtzite (Wz) materials
- Effect of different scattering mechanisms on Carrier's transport
- Non-equilibrium conditions transport parameters can be extracted
- State of Art tool to characterize wafers theoretically in terms of carrier's velocity

## CHAPTER 2

### Start using TNL-EM simulator



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## 2.1 Summary

**TNL-EM simulator** is a purely atomistic physic based three dimensional material mobility characterization simulator. To simulate electronic transport from particles prospective, a well established Ensemble Monte Carlo (EMC) technique is used as a direct simulation of the dynamics of charge carriers inside the crystal under the applied electric field, making it capable to extract the required physical information under non-equilibrium states. The solution of Boltzmann transport equation (BTE) under non-equilibrium includes rate change of distribution function, however under equilibrium, the distribution function resemble with the Fermi-Dirac function. Different scattering mechanisms are responsible for the mobility degradation phenomenon.

**TNL-EM simulator** is capable to predict the accurate drift velocity of specified semiconductor sample and provides insight to model the carrier velocity in terms physical mechanisms associated with the transport of carriers. It helps in characterizing epi-wafers before processing, and is a state of art tool to model carrier velocity theoretically.

**TNL-EM simulator** can be worked as standalone tool as well as in interfaced environment through conjunction with TNL-FB simulator. It is user friendly simulator, users will find easy to learn hands on working on **TNL-EM simulator**.

### 2.1.1 The Graphical User Interface

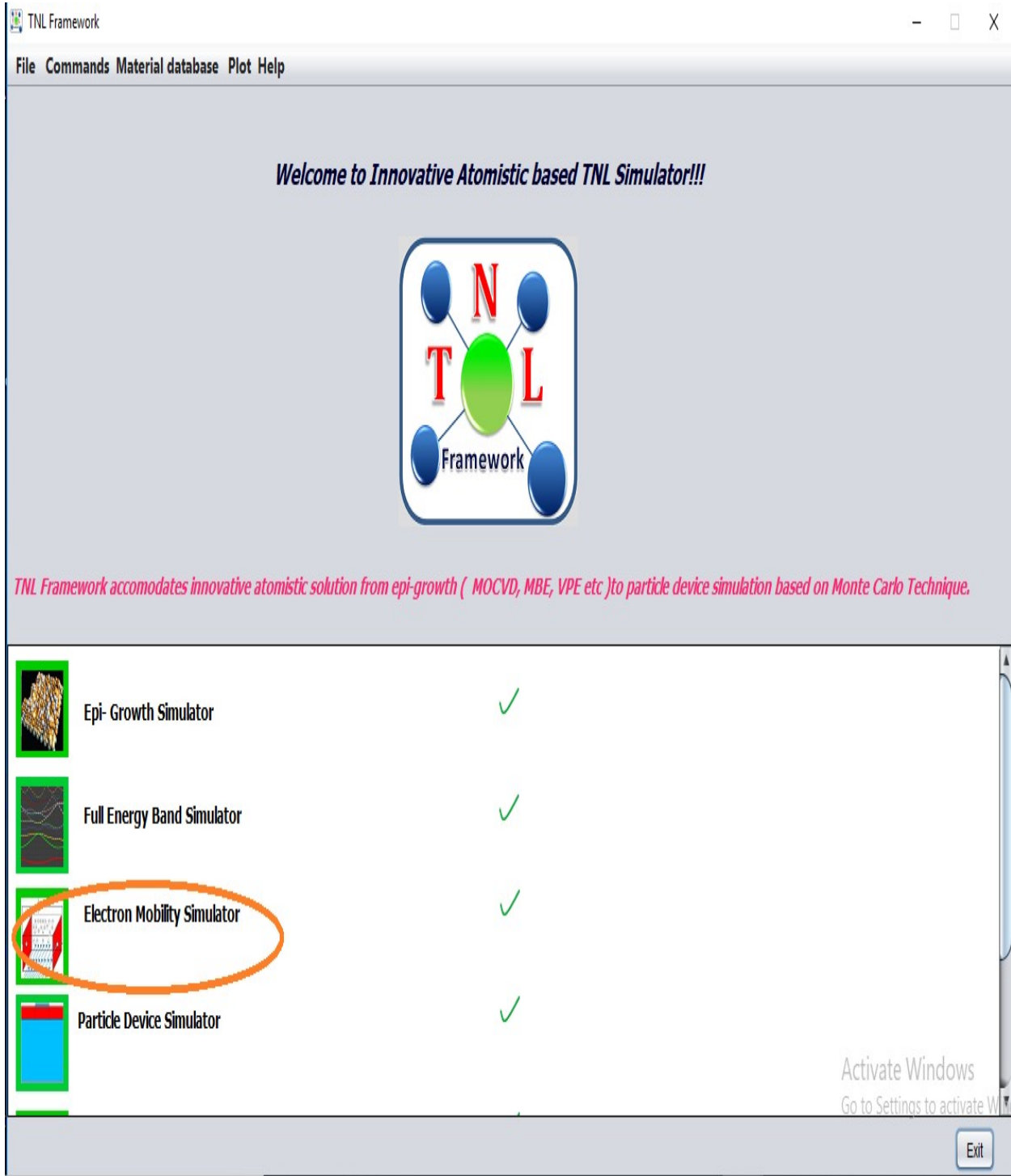
The graphical user interface (GUI) capabilities of of **TNL-EM simulator** extend a convenient and comfortable approach to users for characterization of the carrier velocity under external electric field, choosing inbuilt appropriate physical scattering models and running the simulations. The run output window allows users to check the initial data provided by them and analyzing the results. The output data in text file and plot file associated with even single electron can be saved at user's defined locations.

### 2.1.2 Start Using of TNL-EM simulator

The GUI feature of **TNL-EM simulator** is interfaced to the Atomistic TNL Framework and takes advantage of the framework environment. It can work in Stand-alone mode as well as interfaced mode with family of TNL simulators.

The hand's on tutorial is as follows:

Open TNL framework and double click on of **TNL-EM simulator** shown below:



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TNL-EM simulator frame will be open as shown below:

The screenshot displays the TNL-EM simulator interface. The window title is "ELECTRON MOBILITY SIMULATOR". The interface is divided into two main sections: "Material Parameter" and "Scattering Mechanism".

**Material Parameter Section:**

- Choose Material:
- Temp:
- Magnetic Field:
- Electric Field-X:
- Electric Field-Y:
- Electric Field-Z:
- Density:
- Sound Velocity:
- Non Parabolicity:
- G-valley effective mass:
- L-valley effective mass:
- X-valley effective mass:
- Relative permittivity (static):
- Relative permittivity High Freq:

**Scattering Mechanism Section:**

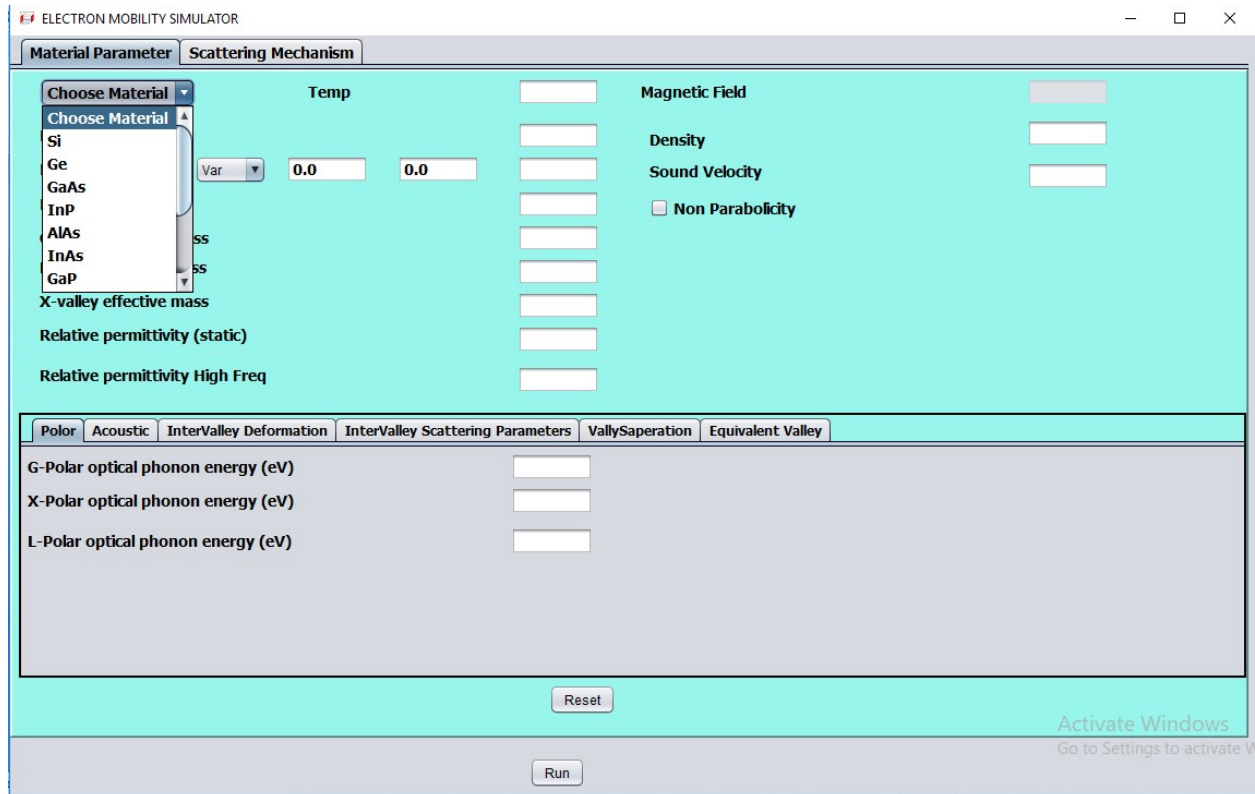
- Polar:
- G-Polar optical phonon energy (eV):
- X-Polar optical phonon energy (eV):
- L-Polar optical phonon energy (eV):

At the bottom of the interface, there are two buttons: "Reset" and "Run". A watermark "Activate Windows" is visible in the bottom right corner.

of TNL-EM simulator frame consists of two sub windows with name Material Parameters and Scattering Mechanisms.

### 2.1.3 Material Parameters

**TNL-EM simulator** includes various cubic, zinblende and wurtzite semiconductor materials database. Under *Material Parameters* frame window have several option to choose appropriate material to run the simulation. All the other material parameters will be filled automatically at appropriate material parameters locations in the frame after choosing the material. Users have flexibility to change their own material parameters by changing the default material parameter value loaded for material chosen at appropriate location. The lower half of of **TNL-EM simulator** frame consist of other specific material parameters required to run particle based simulation. The description of each material parameter in upper and lower half of of **TNL-EM simulator** frame is given below:



The elemental and compound semiconductor materials databases are by default in TNL database for **TNL-EM simulator**.

After choosing material and temperature, user will input the value electric field require to analyze their sample. In general practice, y direction the variable electric field has been applied.

User will input the effective mass of carrier at gamma, L and X valley, which can be extracted from the TNL-FB simulator. The relative permittivity for static and high frequency permittivity will be fill in next step.

On right hand side of the **TNL-EM simulator** frame, user has option to provide value of magnetic field to analyze Hall effects on the sample. (In current version the application of magnetic field B option is kept hide, next version will include effect of magnetic field as well).

The density and sound velocity of the sample will be inputted in next step. User has flexibility to choose the carrier transport on non-parabolic bands by just checking the box Non-parabolicity. User may provide non-parabolicity factors values for gamma, L and X valleys.

The screenshot displays the 'ELECTRON MOBILITY SIMULATOR' window. It features two main tabs: 'Material Parameter' and 'Scattering Mechanism'. The 'Material Parameter' tab is active, showing a grid of input fields for various physical properties. The 'Scattering Mechanism' tab is also visible, showing input fields for different scattering parameters. The interface includes a 'Reset' button and a 'Run' button at the bottom. A watermark 'Activate Windows' is visible in the bottom right corner.

Material Parameter	Value	Scattering Mechanism	Value
Choose Material	[Dropdown]	Temp	[Input]
Electric Field-X	[Input]	Magnetic Field	[Input]
Electric Field-Y	[Var] [0.0] [0.0]	Density	[Input]
Electric Field-Z	[Input]	Sound Velocity	[Input]
G-valley effective mass	[Input]	<input checked="" type="checkbox"/> Non Parabolicity	
L-valley effective mass	[Input]	G-valley nonparabolicity	[Input]
X-valley effective mass	[Input]	L-valley nonparabolicity	[Input]
Relative permittivity (static)	[Input]	X-valley nonparabolicity	[Input]
Relative permittivity High Freq	[Input]		
Polar		Equivalent Valley	
G-Polar optical phonon energy (eV)	[Input]		
X-Polar optical phonon energy (eV)	[Input]		
L-Polar optical phonon energy (eV)	[Input]		

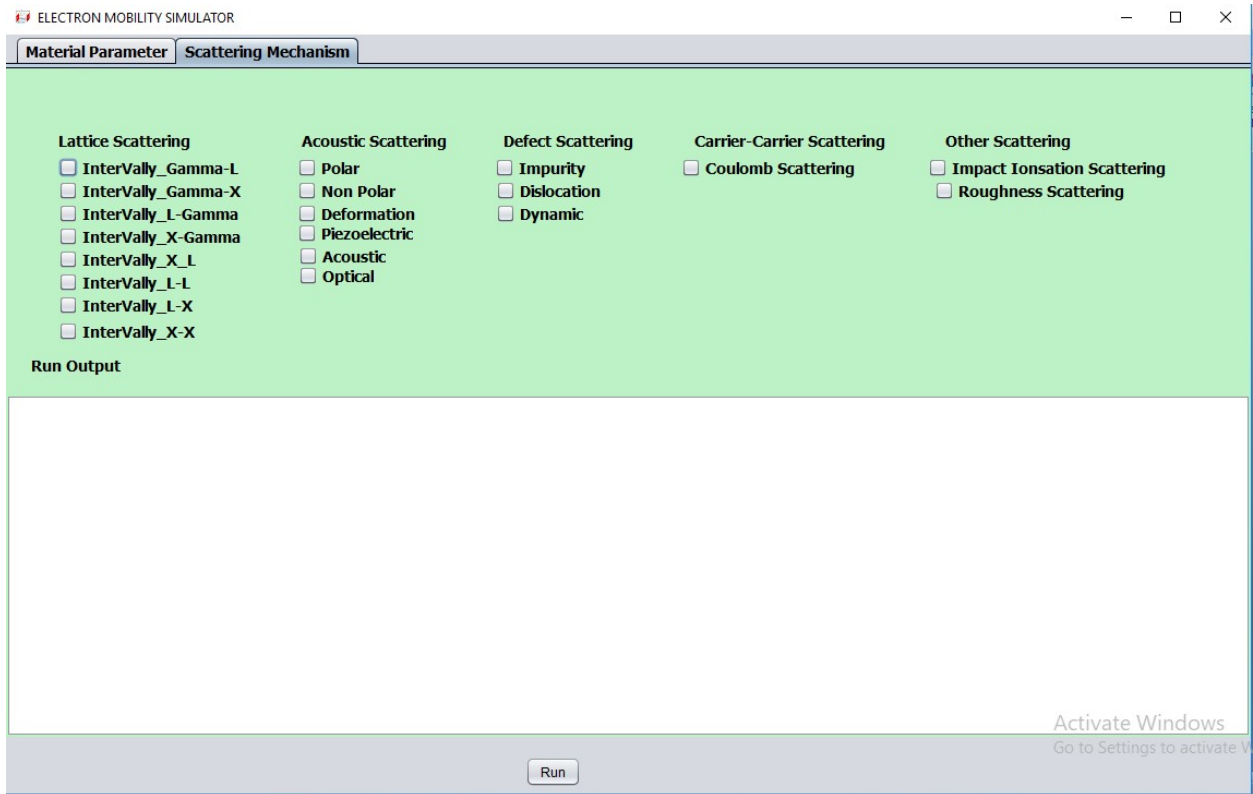
At below in the frame, user need to fill values different energies, deformation potentials, scattering parameters and number equivalent valleys in different directions, energy separations values between different valleys etc. All these parameters can be extracted from the full electronic band structure through **TNL-FB simulator**.

Alternatively, users may find these above parameters values reported by others from the link:

<http://www.ioffe.ru/SVA/NSM/Semicond/>

## 2.1.4 Scattering Mechanisms

The upper portion of other sub window in **TNL-EM simulator** frame is for choosing different types scattering mechanisms to invoke particular scattering in the electronic transport simulation through solution of Boltzmann transport equation (BTE).



The lower portion of other sub window in **TNL-EM simulator** frame is run output window to show output of simulation running status.



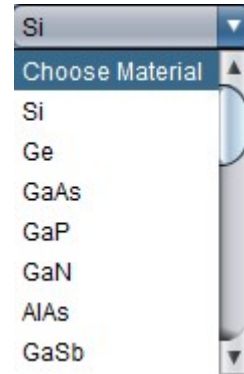
## 2.2 Hands on Tutorial:

For new user to get familiar with TNL Electron Mobility Simulator, user may follow step by step the given tutorial.

In current tutorial, the Gallium Arsenide (GaAs) wafer is chosen for wafer characterisation in terms drift velocity exploiting the TNL Electron Mobility Simulator.

### 2.2.1 Choose Material

- Invoke TNL Electron Mobility Simulator using Framework.
- Choose Material parameter Tab from top-left side
- In present case “GaAs” is needed for simulation.
- Click on Choose Material Button.
- Choose “GaAs” for Simulation.



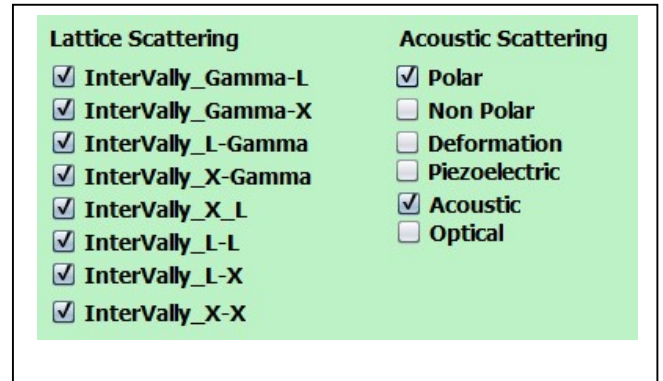
### 2.2.2 Material Parameter

- Temperature is by default 300°K.
- Set Electric Field in X Direction 0.0.
- Set Electric field variable in Y Direction,
- Initial electric field in 0.0, Step Size 1.0.
- Final Electric Field in Y Direction 7.0.
- Make sure all material parameter are filled by just clicking on each button

GaAs	Temp	300	Magnetic Field																									
Electric Field-X		0.0	Density	5370.0																								
Electric Field-Y	Var	0.0 1.0	7	Sound Velocity	5.22E3																							
Electric Field-Z		0	<input type="checkbox"/> Non Parabolicity																									
G-valley effective mass		0.063																										
L-valley effective mass		0.170																										
X-valley effective mass		0.58																										
Relative permittivity (static)		12.9																										
Relative permittivity High Freq		10.92																										
<table border="1"> <tr> <td>Polar</td> <td>Acoustic</td> <td>InterValley Deformation</td> <td>InterValley Scattering Parameters</td> <td>VallySaperation</td> <td>Equivalent Valley</td> </tr> <tr> <td>G-Polar optical phonon energy (eV)</td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>X-Polar optical phonon energy (eV)</td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>L-Polar optical phonon energy (eV)</td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> </table>					Polar	Acoustic	InterValley Deformation	InterValley Scattering Parameters	VallySaperation	Equivalent Valley	G-Polar optical phonon energy (eV)						X-Polar optical phonon energy (eV)						L-Polar optical phonon energy (eV)					
Polar	Acoustic	InterValley Deformation	InterValley Scattering Parameters	VallySaperation	Equivalent Valley																							
G-Polar optical phonon energy (eV)																												
X-Polar optical phonon energy (eV)																												
L-Polar optical phonon energy (eV)																												

### 2.2.3 Scattering Mechanism

- Click on Scattering Mechanism tab.
- Select all Lattice Scattering i.e.,
- Select Intervalley Gama-L.
- Select Intervalley Gama-X.
- Select Intervalley L-Gama.
- Select Intervalley X-Gama.
- Select Intervalley X-L.
- Select Intervalley L-L.
- Select Intervalley X-X.
- Select Polar Scattering.
- Select Acoustic Scattering.

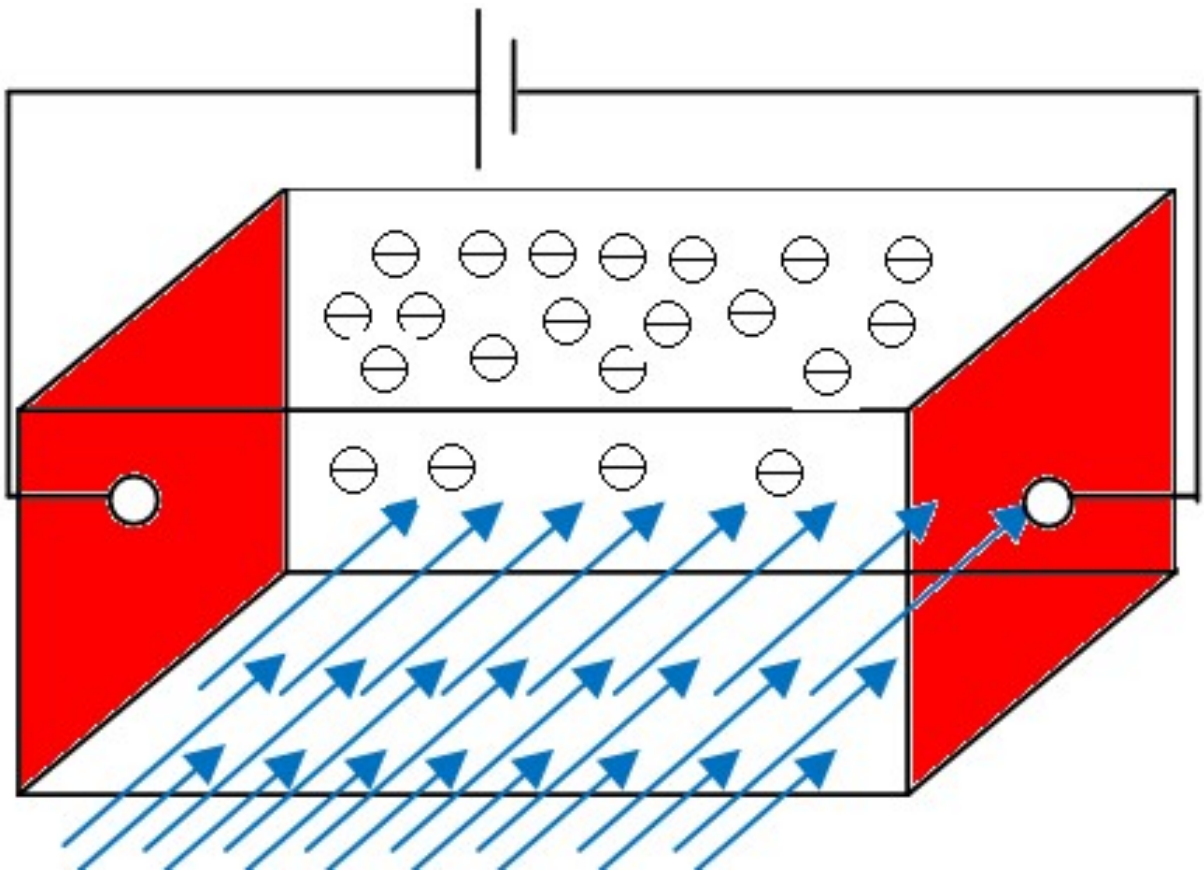


### 2.2.4 Output

- All the run output data will be stored at specified location by users. User need to click on “Run” button.
- Check run time Output at in “Run Output” window at bottom of Scattering Mechanism tab.
- Simulated output data can be plotted in “.plot” format, can be plotted in TNLPlot.

# CHAPTER 3

## Physics



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### 3.1 Introduction

**TNL-EM simulator** uses Monte Carlo technique to simulate the transport properties of n- and p-type different semiconductor materials at user defined temperature in crossed electric and magnetic fields. The electric field dependence of the distribution function, mobility, electron mean energy, population ratio, average drift velocity, Hall angle, and Hall coefficient can be investigated in details.

The **TNL-EM simulator** calculate hot electron transport properties in semiconductors with the approached by attempting to solve the Boltzmann transport equation to derive the distribution function for the charge carriers. However, the integro-differential form of this equation usually makes it necessary to introduce rather severe approximations to obtain a solution, particularly when non-randomizing, inelastic collisions are to be considered. For this reason a Monte Carlo technique, the accuracy of which is limited only by the physical model adopted for the scattering rates and full band structure, has been first used by Kurosawa [1]. This technique has been generalized by Boardman et al. [2] and Fawcett et al. [3] later by easing the incorporation of complicated scattering processes and band structure scan.

The scope of the Monte Carlo method in **TNL-EM simulator** can be simply extended to include the cases where external electric fields are present. It is then possible to calculate, the carrier mobility of a semiconductor as functions of electric field strengths [4].

### 3.2 Boltzmann Transport Model

The **TNL-EM simulator** includes basic technique as applied to transport problems is to simulate the free particle motion (referred to as the free flight) which can be terminated by instantaneous random scattering events. The Monte Carlo algorithm implemented in **TNL-EM simulator** consists of generating random free flight times for each particle, choosing the type of scattering occurring at the end of the free flight, changing the final energy and momentum of the particle after scattering, and then repeating the procedure for the next free flight. Sampling the particle motion at various times throughout the simulation allows for the statistical estimation of physically interesting quantities such as the single particle distribution function, the average drift velocity in the presence of an applied electric field, the average energy of the particles, *etc.* By simulating an *ensemble* of particles in **TNL-EM simulator**, representative of the physical system of interest, the non-stationary time-dependent evolution of the electron and hole distributions under the influence of a time-dependent driving force may be simulated.

This particle-based picture, in which the particle motion is decomposed into free flights terminated by instantaneous collisions, is basically the same approximate picture underlying the derivation of the semi-classical Boltzmann Transport Equation (BTE). In fact, it may be shown in **TNL-EM simulator** that the one-particle distribution function obtained from the random walk Monte Carlo technique satisfies the BTE for a homogeneous system in the long-time limit.

The **TNL-EM simulator** considers, BTE through a region of phase space about the points  $(x, y, z, p_x, p_y, p_z)$ . The number of particles entering this region in time  $dt$  is equal to the number which were in the region of phase space  $(x-v_x dt, y-v_y dt, z-v_z dt, p_x-F_x dt, p_y-F_y dt, p_z-F_z dt)$  at a time  $dt$  earlier. The  $f(x, y, z, p_x, p_y, p_z)$  is the distribution function which expresses the number of particles per quantum state in the region, then the change  $df$  which occurs during time  $dt$  due to the motion of the particles in coordinate space and due to the fact that force fields acting on the particles tend to move them from one region to another in momentum space is [5] – [10]:

$$df = f(x - v_x dt, y - v_y dt, z - v_z dt, p_x - F_x dt, p_y - F_y dt, p_z - F_z dt) - f(x, y, z, p_x, p_y, p_z) \quad (3.1)$$

Using Taylor series expansion, we get

$$\frac{df}{dt} = -\mathbf{v} \cdot \nabla_r f - \mathbf{F} \cdot \nabla_p f \quad (3.2)$$

Only the change in the distribution function due to the motion of particles in coordinate space and due to the momentum changes arising from the force fields acting on the particles have been accounted for in **TNL-EM simulator**. Particles may also be transferred into or out of a given region in phase space by collisions or scattering interactions involving other particles of the distribution or scattering centers external to the assembly of particles under consideration. If the rate of change of the distribution function due to collisions, or scattering, is denoted by

$(\partial f / \partial t)_{coll}$ , the total rate of change of  $f$  becomes

$$\frac{df}{dt} = -\mathbf{v} \cdot \nabla_r f - \mathbf{F} \cdot \nabla_p f + \left. \frac{\partial f}{\partial t} \right|_{coll} + s(r, p, t) \quad (3.3)$$

$$\frac{df}{dt} + \mathbf{v} \cdot \nabla_r f + \mathbf{F} \cdot \nabla_p f = \left. \frac{\partial f}{\partial t} \right|_{coll} + s(r, p, t) \quad (3.4)$$

The last term on the RHS of Eq. (3.3) and (3.4) is the generation-recombination processes which play significant role. The Eq. (3.4) represents the Boltzmann transport equation for the particle flow in the phase space. The various terms in Eq. (3.4) is describing below.

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The last term on the LHS of Eqs. (3.4) is

$$(\partial f / \partial t)_{forces} = -\mathbf{F} \cdot \nabla_{\mathbf{p}} f, \quad (3.5)$$

The total force equals the sum of the force due to the Lorentz force i.e. due to electric field  $\mathbf{E}$  and the magnetic flux density,  $\mathbf{B}$  and can be given as.

$$\mathbf{F} = \frac{d\mathbf{p}}{dt} = \hbar \frac{d\mathbf{k}}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \quad (3.6)$$

The second term on the LHS of Eqs. (3.4) is given as

$$(\partial f / \partial t)_{diff} = -\mathbf{v} \cdot \nabla_{\mathbf{r}} f. \quad (3.7)$$

This term arises if there is a spatial variation in the distribution function due to concentration or temperature gradients, both of which will result in a diffusion of carriers in coordinate space.

The first term on the RHS of Eqs. (3.4)  $(\partial f / \partial t)_{coll}$  is the collision term which equals the difference between the in-scattering and the out-scattering processes, and is given as

$$\left( \frac{\partial f}{\partial t} \right)_{coll} = \sum_{k'} \{ S(\mathbf{k}', \mathbf{k}) f(\mathbf{k}') [1 - f(\mathbf{k})] - S(\mathbf{k}, \mathbf{k}') f(\mathbf{k}) [1 - f(\mathbf{k}')] \} = \widehat{C}f \quad (3.8)$$

The presence of  $f(\mathbf{k})$  and  $f(\mathbf{k}')$  in the collision integral makes the BTE rather complicated integro-differential equation for  $f(\mathbf{r}, \mathbf{k}, t)$ , whose solution requires a number of simplifying assumptions. In the absence of perturbing fields and temperature gradients, the distribution function must be the Fermi-Dirac function. In this case, the collision term must vanish and the principle of detailed balance gives for all  $\mathbf{k}$  and  $\mathbf{k}'$  and all scattering mechanisms

$$\frac{S(\mathbf{k}, \mathbf{k}')}{S(\mathbf{k}', \mathbf{k})} = \frac{f_0(\mathbf{k}') [1 - f_0(\mathbf{k})]}{f_0(\mathbf{k}) [1 - f_0(\mathbf{k}')]}. \quad (3.9)$$

Therefore, if the phonons interacting with the electrons are in thermal equilibrium, we get

$$\frac{S(\mathbf{k}, \mathbf{k}')}{S(\mathbf{k}', \mathbf{k})} = \exp\left(\frac{E_{\mathbf{k}} - E_{\mathbf{k}'}}{k_B T}\right). \quad (3.10)$$

This relation must be satisfied regardless of the origin of the scattering forces. If, for example, we assumed  $E_{\mathbf{k}} > E_{\mathbf{k}'}$ , then  $S(\mathbf{k}, \mathbf{k}')$  which involves emission must exceed  $S(\mathbf{k}', \mathbf{k})$  which involves absorption. Note that the BTE is valid under assumptions of semi-classical transport: effective mass approximation (which incorporates the quantum effects due to the periodicity of

the crystal); Born approximation for the collisions, in the limit of small perturbation for the electron-phonon interaction and instantaneous collisions; no memory effects, i.e. no dependence on initial condition terms. The phonons are usually treated as in equilibrium, although the condition of non-equilibrium phonons may be included through an additional equation.

### 3.3 Scattering Models

The total scattering rate  $\Gamma_j$  is a sum of all possible scattering rates. For computational technical reasons each scattering mechanism in **TNL-EM simulator** has been numbered sequentially from one to  $N_r$ , the total number of such mechanisms considered. Once the numbering has been decided it should not change during simulation. The total scattering rate is

$$\Gamma[\mathbf{k}(t)] = \sum_{i=1}^{N_r} \lambda_i[\mathbf{k}(t)] \quad (3.11)$$

where  $t$  represents time, which is related to the energy or wave vector of the scattering particle through Equations (3.11), and  $\lambda_i$  the rate of scattering mechanism  $i$ . The scattering mechanism terminating the free flight is selected by means of a random number.

$$r_\gamma = \Gamma r_s \quad (3.12)$$

where  $r_s$  represents a flat random number.

Free carriers (electrons and holes) interact with the crystal and with each other through a variety of scattering processes which relax the energy and momentum of the particle. Based on first order, time-dependent perturbation theory, the transition rate from an initial state  $\mathbf{k}$  in band  $n$  to a final state  $\mathbf{k}'$  in band  $m$  for the  $j^{\text{th}}$  scattering mechanism is given by Fermi's Golden rule [11].

$$\Gamma_j[n, \mathbf{k}; m, \mathbf{k}'] = \frac{2\pi}{\hbar} \left| \langle m, \mathbf{k}' | V_j(\mathbf{r}) | n, \mathbf{k} \rangle \right|^2 \delta(E_{\mathbf{k}'} - E_{\mathbf{k}} \mp \hbar\omega) \quad (3.13)$$

where  $V_j(\mathbf{r})$  is the scattering potential of this process,  $E_{\mathbf{k}}$  and  $E_{\mathbf{k}'}$  are the initial and final state energies of the particle. The delta function describes conservation of energy, valid for long times after the collision is over, with  $\hbar\omega$  the energy absorbed (upper sign) or emitted (lower sign) during the process. The total scattering rate used to generate the free flight is given by

$$\Gamma_j[n, \mathbf{k}] = \frac{2\pi}{\hbar} \sum_{m, \mathbf{k}'} \left| \langle m, \mathbf{k}' | V_j(\mathbf{r}) | n, \mathbf{k} \rangle \right|^2 \delta(E_{\mathbf{k}'} - E_{\mathbf{k}} \mp \hbar\omega). \quad (3.14)$$

The scattering rates  $\Gamma_j[n, \mathbf{k}; m, \mathbf{k}']$  and  $\Gamma_j[n, \mathbf{k}]$  are calculated using time dependent perturbation theory using Fermi's rule, Eqs. (3.13) and (3.14), and the calculated rates are then tabulated in a

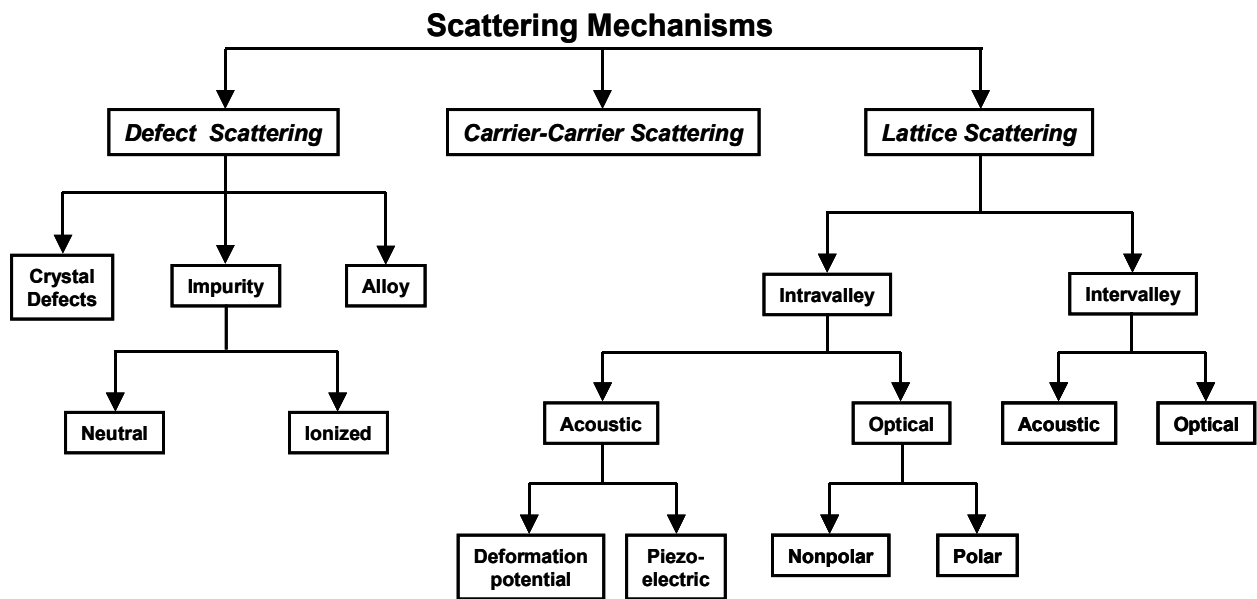
scattering table in order to select the type of scattering and final state after scattering as discussed earlier. The scattering mechanism  $j$  is selected satisfying the inequality from the equation (3.12):

$$\sum_{i=1}^{j-1} \lambda_i[k(t)] \leq r_\gamma < \sum_{i=1}^j \lambda_i[k(t)] \quad (3.15)$$

with

$$\sum_{i=1}^0 \lambda_i[k(t)] = 0 \quad (3.16)$$

Thus, the various scattering mechanisms are passed through in the sequence they have been ordered until  $\sum \lambda_i$  exceeds  $r_\gamma$ . The search terminates sooner the smaller the value of  $r_\gamma$  which is we have given the above-mentioned advice on numbering the various scattering mechanisms. This scheme makes a weighted selection such that, over a long period of time, the relative amount of scattering from a particular type equals its fractional part of the total scattering rate or cross-section. The different types of scattering mechanisms is implemented in the **TNL-EM simulator** taken from [3], [7]



**Scattering mechanisms in a typical semiconductor implemented in ElectronMobility Simulator**

The basic formalisms used in **TNL-EM simulator** for scattering events are as above:

- Fraction of all scattering events caused by polar optical phonons against the electric field for each separate minimum.

e = phonon emission

a = absorption



- Fraction of all scattering events during steady state causing transfer of carriers between conduction band minima in zincblende and wurtzite semiconductor materials against the electric field.

Carrier transfer in zincblende:  $\Gamma \rightarrow X$ ,  $L \rightarrow X$  and  $\Gamma \rightarrow L$  valleys

Carrier transfer in wurtzite :  $\Gamma^1 \rightarrow \Gamma^3$ ,  $\Gamma^3 \rightarrow U$  and  $\Gamma^1 \rightarrow U$  valleys

Carrier transfer in the zincblende opposite direction, e.g.  $X \rightarrow \Gamma$ ,  $X \rightarrow L$  and  $L \rightarrow \Gamma$  valleys

Carrier transfer in the wurtzite opposite direction, e.g.  $\Gamma^3 \rightarrow \Gamma^1$ ,  $U \rightarrow \Gamma^3$  and  $U \rightarrow \Gamma^1$  valleys

Here,

$e$  = phonon emission

$a$  = absorption

- Fraction of scattering events during steady state causing transfer within the equivalent X and L minima in zincblende semiconductor materials and  $\Gamma^3$  and U minima in wurtzite semiconductor materials.

$e$  = phonon emission

$a$  = absorption

### 3.4 Free Flight Generation

The **TNL-EM simulator**, particle motion is assumed to consist of free flights terminated by instantaneous scattering events, which change the momentum and energy of the particle after scattering. The first task is to generate free flights of random time duration for each particle. To simulate this process, the probability density,  $P(t)$ , is required, in which  $P(t)dt$  is the joint probability that a particle will arrive at time  $t$  without scattering after a previous collision occurring at time  $t = 0$ , and then suffer a collision in a time interval  $dt$  around time  $t$ . The probability of scattering in the time interval  $dt$  around  $t$  may be written as  $\Gamma[k(t)]dt$ , where  $\Gamma[k(t)]$  is the scattering rate of an electron or hole of wavevector  $k$ . The scattering rate,  $\Gamma[k(t)]$ , represents the sum of the contributions from each individual scattering mechanism, which are usually calculated quantum mechanically using perturbation theory, as described later. The implicit dependence of  $\Gamma[k(t)]$  on time reflects the change in  $k$  due to acceleration by internal and external fields. For electrons subject to time independent electric and magnetic fields, Eq. 3.6 may be integrated to give the time evolution of  $k$  between collisions as [7]

$$\mathbf{k}(t) = \mathbf{k}(0) - \frac{e(\mathbf{E} + \mathbf{v} \times \mathbf{B})t}{\hbar} \quad (3.17)$$

where  $\mathbf{E}$  is the electric field,  $\mathbf{v}$  is the electron velocity is given by  $\mathbf{v} = \frac{1}{\hbar} \frac{d\epsilon}{d\mathbf{k}}$ , and  $\mathbf{B}$  is the magnetic flux density. In terms of the scattering rate,  $\Gamma[\mathbf{k}(t)]$ , the probability that a particle has

not suffered a collision after a time  $t$  is given by  $\exp\left(-\int_0^t \Gamma[\mathbf{k}(t')] dt'\right)$ . Thus, the probability of scattering in the time interval  $dt$  after a free flight of time  $t$  may be written as the joint probability

$$P(t)dt = \Gamma[\mathbf{k}(t)] \exp\left[-\int_0^t \Gamma[\mathbf{k}(t')] dt'\right] dt \quad (3.18)$$

Random flight times may be generated according to the probability density  $P(t)$  above using, for example, the pseudo-random number generator implicit on most modern computers, which generate uniformly distributed random numbers in the range  $[0,1]$ . Using a direct method, random flight times sampled from  $P(t)$  may be generated according to [7]

$$r = \int_0^{t_r} P(t) dt \quad (3.19)$$

where  $r$  is a uniformly distributed random number and  $t_r$  is the desired free flight time. Integrating Eq. (3.19) with  $P(t)$  given by Eq. (3.18) above yields [7]

$$r = 1 - \exp\left[-\int_0^{t_r} \Gamma[\mathbf{k}(t')] dt'\right] \quad (3.20)$$

Since  $1 - r$  is statistically the same as  $r$ , Eq. (3.20) may be simplified to

$$-\ln r = \int_0^{t_r} \Gamma[\mathbf{k}(t')] dt' \quad (3.21)$$

Eq. (3.21) is the fundamental equation used to generate the random free flight time after each scattering event, resulting in a random walk process related to the underlying particle distribution function. If there is no external driving field leading to a change of  $\mathbf{k}$  between scattering events the time dependence vanishes, and the integral is trivially evaluated. In the general case where this simplification is not possible, it is expedient to introduce the so called self-scattering method in which we introduce a fictitious scattering mechanism whose scattering rate always adjusts

itself in such a way that the total (self-scattering plus real scattering) rate is a constant in time [12].

$$\Gamma = \Gamma[\mathbf{k}(t')] + \Gamma_{self}[\mathbf{k}(t')] \quad (3.22)$$

where  $\Gamma_{self}[\mathbf{k}(t')]$  is the self-scattering rate. The self-scattering mechanism itself is defined such that the final state before and after scattering is identical. Hence, it has no effect on the free flight trajectory of a particle when selected as the terminating scattering mechanism, yet results in the simplification of Eq. (3.20) such that the free flight is given by

$$t_r = -\frac{1}{\Gamma} \ln r \quad (3.23)$$

The constant total rate (including self-scattering)  $\Gamma$ , must be chosen at the start of the simulation interval (there may be multiple such intervals throughout an entire simulation) so that it is larger than the maximum scattering encountered during the same time interval. In the simplest case, a single value is chosen at the beginning of the entire simulation (constant gamma method), checking to ensure that the real rate never exceeds this value during the simulation. Other schemes may be chosen that are more computationally efficient, and which modify the choice of  $\Gamma$  at fixed time increments.

### 3.5 Choice of Scattering Angles

Defining a spherical coordinate system around the initial wavevector  $\mathbf{k}$ , the final wavevector  $\mathbf{k}'$  is specified by  $|\mathbf{k}'|$  (which depends on conservation of energy) as well as the azimuthal and polar angles,  $\varphi$  and  $\theta$  around  $\mathbf{k}$ . Typically, the scattering rate,  $\Gamma_j[n, \mathbf{k}; m, \mathbf{k}']$ , only depends on the angle  $\theta$  between  $\mathbf{k}$  and  $\mathbf{k}'$ . Therefore,  $\varphi$  may be chosen using a uniform random number between 0 and  $2\pi$  (i.e.  $2\pi r$ ), while  $\theta$  is chosen according to the angular dependence for scattering arising from  $\Gamma_j[n, \mathbf{k}; m, \mathbf{k}']$ . If the probability for scattering into a certain angle  $P(\theta)d\theta$  is integrable, the random angles satisfying this probability density may be generated from a uniform distribution between 0 and 1 through inversion of Eq. (3.19) [7].

Once the scattering mechanism has been selected, the scattering angles have to be calculated in order to determine the initial direction of the next flight. ElectronMobility simulator takes into account the polar angular dependence of the scattering rate of electrons in a prototypical polar semiconductor, due to polar optical phonon scattering. The probability density for scattering into an angle  $\theta$ , relative to the original trajectory of travel just before scattering, is given by [7]

$$P(\theta)d\theta = \frac{\Gamma_{POP}(\theta)d\theta}{\int_0^\pi \Gamma_{POP}(\theta)d\theta} \sim \frac{\sin(\theta)d\theta}{(E + E' - 2\sqrt{EE'} \cos\theta)} \quad (3.24)$$

where  $\Gamma_{POP}(\theta)$  is the scattering rate into a small angle  $d\theta$  around the angle  $\theta$ ,  $E$  is the energy of the particle before scattering, and  $E' = E \pm \hbar\omega_o$  is the final energy corresponding to the emission (lower sign) or absorption (upper sign) of an optical phonon of energy  $\hbar\omega_o$ . The integral in the numerator is for normalization.

### 3.6 Ensemble Monte Carlo Simulation

The basic Monte Carlo algorithm implemented in **TNL-EM simulator** is described above may be used to track a single particle over many scattering events in order to simulate the steady-state behavior of a system. However, for improved statistics over shorter simulation times, and for transient simulation, the preferred technique is the use of a *synchronous ensemble* of particles, in which the basic Monte Carlo algorithm is repeated for each particle in a ensemble representing the (usually larger) system of interest until the simulation is completed. Since there is rarely an identical correspondence between the number of simulated charges, and the number of actual particles in a system, each particle is really a *super-particle*, representing a finite number of real particles. The corresponding charge of the particle is weighted by this super-particle number. In **TNL-EM simulator** each carrier is simulated only up to the end of the time-step, and then the next particle in the ensemble is treated. Over each time step, the motion of each particle in the ensemble is simulated independent of the other particles. Nonlinear effects such as carrier-carrier interactions or the Pauli Exclusion Principle are then updated at each times step, as discussed in more detail below.

The non-stationary one-particle distribution function and related quantities such as drift velocity, valley or subband population, etc., are then taken as averages over the ensemble at fixed time steps throughout the simulation. For example, the drift velocity in the presence of the field is given by the ensemble average of the component of the velocity at the  $n$ th time step as

$$\bar{v}_z(n\Delta t) \cong \frac{1}{N} \sum_{j=1}^N v_z^j(n\Delta t), \quad (3.25)$$

where  $N$  is the number of simulated particles and  $j$  labels the particles in the ensemble. This equation represents an estimator of the true velocity, which has a standard error given by

$$s = \frac{\sigma}{\sqrt{N}} \quad (3.26)$$

where  $\sigma^2$  is the variance which may be estimated from

$$\sigma^2 \cong \frac{N}{N-1} \left\{ \frac{1}{N} \sum_{j=1}^N (v_z^j)^2 - \bar{v}_z^2 \right\}. \quad (3.27)$$

Similarly, the distribution functions for electrons and holes may be tabulated by counting the number of electrons in cells of  $k$ -space. From Eq. (3.26), we see that the error in estimated average quantities decreases as the square root of the number of particles in the ensemble, which necessitates the simulation of many particles. Typical ensemble sizes for good statistics are in the range of  $10^4 - 10^6$  particles.

**Note:** In current version of software users can simulate the effect of external Electric field only through in **TNL-EM simulator**. The motion of carriers in external Electro-magnetic field is due in next version of the software to analyze Hall mobility and extracting  $R_H$ .

Users are refer to [http://www.technextlab.com/Scientific\\_Report\\_Nature.pdf](http://www.technextlab.com/Scientific_Report_Nature.pdf) for more further details of **TNL-EM simulator** and its capabilities.

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