Chapter 2
MONTE CARLO SIMULATIONS

2.1 Principles

The Monolithic Microwave Integrated Circuit (MMIC) technologies based on Metal Semiconductor Field Effect Transistors (MESFET) and High Electron Mobility Transistors (HEMT) for 40 GHz operations require a gate length of 0.25 micron. Currently electron beam (E-beam) lithography is used to define gate length of 0.25 micron or lower. It is desirable to develop fundamental understanding of interaction of electron beam with resist, used to define the gate, and substrate over which the resist is coated. It is necessary to understand lithography parameters, like sensitivity, thoroughly before direct write and development of the gate features is carried out on a wafer. Presently in Solid State Physical Laboratory (SSPL) an experimental approach is used to develop a process for direct writing of 0.25 micron gate. Sets of experiments are carried out first to characterize e-beam resist for sensitivity and contrast. Then, next, exposure dose and development time are varied to arrive at a process for defining the gate. The outcome of the experimental work is influenced by other parameters like variability in machine performance and writing strategy. This approach works well but is time consuming and costly. Also in this approach it is not possible to develop an understanding of electron beam energy deposition in the resist and the substrate. For e-beam direct write technology maturity and better understanding of interplay of various parameters, it is necessary to do develop modeling process using Monte - Carlo simulations before carrying out direct write exposures.

Monte Carlo method was pioneered by von Neumann and Ulam in 1915 as a mathematical method to solve the atoms determinable problem by using random numbers. Nowadays it finds wide applications to almost all the fields of physics to investigate both the determinable and primarily stochastic problem. It has also stimulated the various simulation techniques with modern computer to reproduce artificially the phenomena rarely happened by nature, or to obtain the physical quantities which are extremely difficult to derive by other methods. The problem of particle transportation in matter belongs to the later category.
Experimentally, one can measure something resulted from the interaction of electrons with a sample, under the primary electron beam bombardment. Somehow, this interaction process remains as a black box due to the limitation of the present experimental techniques. This then requires a theoretical investigation for deriving information unattainable experimentally. Monte Carlo simulation may be the most powerful theoretical method towards this end, and it also provides a physical insight to the details of interaction processes in addition to their results, while the analytical method like the solving of Boltzmann equation is insufficient to accommodate the complexity of the interaction process and arbitrary boundary condition, which can be easily incorporated into a Monte Carlo model. A simulation itself is, in fact, an idealized experiment. The interpretation of the data gained from the simulation provides the understanding of the phenomena under investigation. Nevertheless, one should note that a simulation is, at the utmost, a technique not for exploring the fundamental laws and principles of the interaction but, inversely, depending on them. Furthermore, a simulation code gets its value only after that some of the calculated results have been compared with the experimental measurement and the agreement is found. We shall follow this principle, and always try to make some comparison with the experiment before a certain kind of calculation being performed.

The Monte Carlo simulation of electron transport is based on the stochastic describing of the scattering process. An electron propagation in a solid is approximated to a classical zigzag trajectory. The turning location at which the electron changes its moving direction is the position where the electron is scattered. Particular values of scattering angle, loss energy, etc., in an individual event are realized by random numbers, according to certain formulas describing the scattering behavior. A huge number of electron trajectories then statistically and dynamically replicates the complex combination of those formulas. We can extract the interested information by summing up the data derived from the history of each electron trajectory. Of course, a large population of electrons is necessary to depress the statistical fluctuations inhered in data.

Therefore, what formulas shall we use and what assumptions shall we make influence the simulation results significantly, but in a manner we can predict when having gained enough experience. This suggests the importance of the model employed, the details of which will be discussed later. We shall suppose that a sample is homogeneous in chemical
composition and amorphous in structure. The assumption of amorphous-like sample is necessary, at the present time, since we approximate the scattering centers randomly distributed within the interaction range of electrons, corresponding to the neglect of diffraction of electron wave by crystal lattice. Furthermore, this ideal amorphous-like sample differs from a real amorphous on that the short-range order are also omitted. This approximation is valid so long as the interaction volume is much greater than the grain size of a polycrystal sample and the electron backscattering from a bulk sample is concerned, since the diffraction effect is smeared out by multiple scattering effect. This diffraction effect can be, in principle, included into Monte Carlo simulation by, for instance, employing Bloch waves derived from the dynamical diffraction theory instead of the simple plane wave which is treated as a particle in the conventional Monte Carlo approach, allowing the extension of the simulation to a crystal [84-85].

The stochastic description of electron collision benefits the concept of scattering cross-section provided by either classical or quantum mechanics. A cross-section is by itself defined as a statistical quantity, being the probability of a dimension of area that an electron would be scattered. In other words, it is a target area statistically meaningful, that an electron would effectively see. When a flux of electrons impact a target the differential cross-section represents a probability distribution.

The concept of electron trajectory borrows the particle picture in classical physics, while a quantum electron is described by the wave function. Usually, an electron is specified by its eigenvalue of momentum, so as to kinetic energy, hence, uncertainty principle prohibits the complete determination of both momentum and position, even though the concept of probability wave and mean free path in quantum mechanics principally allows the statistical modeling, like Monte Carlo simulation, of scattering events possible. The problem is, exactly speaking, we should firstly perform the simulation in momentum space, k-space, other than in real space, r-space, and then transform a particular scattering point into real space through a wave packet, $\Psi_k(r)$ if we are interested in the distribution in real space. In fact, k-space is the basis space for the Monte Carlo simulation in the field as to investigate hot electron transport in semiconductors [86]. But this has not been done yet for the Monte Carlo simulation as applied to electron spectroscopy and microscopy since, historically, one treated electron beam of high energy at least in the order of 10 keV so that the electron wavelength, $\sim 0.12 \, \text{Å}$, is much smaller than the lattice constant. Thus, the particle description has
worked very well.

2.2 Models

A model of electron scattering, depending on our knowledge about the microscopic mechanism of electron interaction, plays an important role on the simulation results. We assume that an electron suffers an elastic scattering only by atomic potential, and an inelastic scattering only through electron-electron interactions. We have come across several models during the course of the research, these models are given as below.

2.2.1 Multiple scattering model.

This model was initiated by Berger [87] for practical Monte Carlo calculations of penetration of charged particles in matter, was based on the use of Bethe’s stopping power equation describing energy loss and angular distributions for electron scattering, which is derived for a certain electron path, s, from the transport equation

\[ f(\theta) = (4\pi)^{-1} \sum_{l=0}^{\infty} (2l + 1) P_l(\cos \theta) \exp \left[ \int_0^s k_i ds \right] \]  

where

\[ k_i = 2\pi N \int_{0}^{\theta} \sigma(\theta) [1 - P_l(\cos \theta)] \sin \theta \ d\theta \]  

with \( P_l(\cos \theta) \) the Legendre polynomial, and \( \sigma(\theta) \) the screened-type Rutherford scattering cross-section. This Model is used in Electron Probe Micro Analysis (EPMA) applications.

2.2.2 Single scattering model.

This model, which is still widely used, adopts the screened Rutherford scattering cross-section \( \sigma_r(\theta) \) in place of the angular distribution \( f(\theta) \) represented by equation (2.1) while the energy loss is given by Bethe’s stopping power equation as in the multiple scattering model. We will be using this model in Elastic scattering simulations and discussing in detail.
### 2.2.3. Hybrid model.

In this model each individual inner-shell ionization was simulated according to Gryzinski’s formulae. The energy loss due to valence electron excitations was imposed on each step length between two individual scattering events in the so-called continuous slowing down approximation, being assessed directly by

\[
\Delta E = \int_0^s \left( -\frac{dE}{ds} \right)_{\text{valance}} ds
\]  

(2.3)

where the stopping power of valence electrons was estimated by the difference of Bethe’s stopping power and the stopping power of the inner-shell electrons, \( \sum_n \left( -\frac{dE}{ds} \right)_n \)

\[
\left( -\frac{dE}{ds} \right)_{\text{valance}} = \left( -\frac{dE}{ds} \right)_{\text{Bethe}} - \sum_n \left( -\frac{dE}{ds} \right)_n
\]

(2.4)

where, according to Bethe,

\[
\left( -\frac{dE}{ds} \right)_{\text{Bethe}} = 2\pi e^4 N \rho \frac{1}{AE} \ln \frac{1.166E}{f}
\]

(2.5)

and, according to Gryzinski,

\[
\left( -\frac{dE}{ds} \right)_n = N \int_{E_n}^{E} (\Delta E) \frac{d\sigma_n}{d(\Delta E)} d(\Delta E)
\]

\[
= \pi e^4 N Z_n \left( \frac{E - E_n}{E + E_n} \right)^{3/2}
\]

\[
\times \left[ \ln \left( \frac{E}{E_n} \right) + \frac{3}{4} \ln \left( 2.7 + \frac{E}{E_n} - 1 \right) \right]
\]

(2.6)

This hybrid model, initially proposed by Schneider and Cormack [88] for the discrete and continuous energy loss processes, has been further developed by some authors (e.g. Berger [87], Reimer and Krefting [89], Shimizu [90], Shimizu and Everhart [91], Ichimura and Shimizu [92], Murata et al [93], Reimer and Stelter [94], and has done much to extend Monte Carlo calculations to alloys and compound materials. We will be discussing this model in detail in inelastic scattering simulations. This model allows the simulation of
the generation of these secondary electrons with high energies and also suited for e-beam lithography applications.

2.2.4. Direct simulation model.

One of the more comprehensive extensions of the hybrid model to an individual inelastic scattering process is to use the individual theoretical stopping powers, for instance, incorporated the differential cross-sections for electron-conduction electron scattering, electron-plasmon scattering and electron-shell electron scattering as follows:

(i) Conduction electron excitation: With respect to the excitation function for conduction electron excitation, this approach has used the excitation function derived by Streitwolf [95],

\[ \sigma_c(E_F) = \frac{0.34 e^4 k_F^2}{3 \pi E_p E_F^2} \]  

(ii) L-shell excitation: According to the semi-quantum-mechanical treatment of Gryzinski [96], the excitation function is written as

\[ \sigma_L(\Delta E) = \frac{\sigma_0}{\Delta E^2} \frac{1}{\Delta E} g_\sigma \left( \frac{E}{\Delta E} \right) \]  

where \( \Delta E, \epsilon \) and \( E \) are the energy loss, minimum energy loss and electron energy, respectively. The angular deflection of primary electrons after the electron-electron interaction is given from the classical binary collision model as

\[ \sin^2 \theta = \frac{\Delta E}{E} \]  

and this was applied to the L-shell electron as well as conduction electron excitations in the present approach.

(iii) Plasmon excitation: Quinn [97] has derived a theoretical expression for the mean free path of a penetrating electron for plasmon excitation, which seems to be most appropriate for the present argument:
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\[ \lambda_p = \frac{2a_o}{\omega_p} E \left( \ln \left( \frac{P^2 + 2m\omega_p}{P - (P^2 - 2\omega_p m)^{1/2}} \right) \right)^{-1} P = (2mE)^{1/2} \quad P_0 = (2mE_F)^{1/2} \quad (2.11) \]

where \( E_F, \omega_p \) and \( a_o \) are the Fermi energy, plasma frequency and Bohr radius, respectively.

It is, from a theoretical viewpoint, probably true that the use of this type of individual inelastic scattering is the most basic approach leading to a more comprehensive understanding of the various excitations associated with electron penetration.

However, this approach requires exact knowledge of individual inelastic scatterings, and this is available for only a few materials, including aluminium. Thus, this leads to a compromise between the direct simulation model and the conventional continuous slowing down approximation, namely to the hybrid model. It should be noted that in both the hybrid and direct simulation models, the Mott scattering cross-section has been used more widely than the screened Rutherford scattering cross-section.

2.2.5. Dielectric function model.

This model is based on use of the Mott scattering cross-section (equation (1.1)) and the dielectric function describing elastic and inelastic processes, respectively. There is no fitting parameter, and the valence electron excitation as well as the inner-shell electron excitation are included exactly according to their oscillator strengths or equivalent energy loss functions. The energy loss distribution and IMFP can be calculated with a double differential cross-section, which also permits the determination of scattering angle. The continuous slowing down approximation is abandoned here, and the simulation can be done for individual inelastic collisions. Furthermore, it is applicable to low-energy electrons as well as to high-energy electrons. The only disadvantages are that the multiple-variable excitation function requires a large amount of memory for a practical computer simulation.

This chapter focus on the simulations for single layer substrates such as Si, GaAs, and PMMA and bi-layer structures such as PMMA on Si and PMMA on GaAs. The complicated calculations of scattering cross sections at the interface of the bi-layer structures is also explained here.
2.3 Monte Carlo Simulations of Single Layer materials:

The Monte-Carlo simulation of electron transport is based on a stochastic description of the scattering process. When an electron impinges on a solid surface it penetrates the solid, undergoing a complicated scattering process. This electron penetration is approximated by classical zigzag trajectory. The location at which the electron changes its direction of movement is the position where the electron is scattered. Particular values of the scattering angle, loss of kinetic energy by the electron, etc., in an individual event are realized by random numbers, according to certain formulae describing the scattering behaviour. The accuracy of the simulation, therefore, depends entirely upon the modeling of these scattering processes, what formulae are used and what assumptions are made, all of which can be predicted when enough knowledge of the process has been gained. Thus a huge number of electron trajectories statistically and dynamically replicates the combination of those formulae, and one can extract the information required by summing up the data derived from the history of each electron trajectory. Further assumptions of practical importance are that a sample is homogeneous in chemical composition and amorphous in structure. The latter is particularly necessary for Monte-Carlo simulation, because we assume that the scattering centers are randomly distributed within the interaction range of electrons.

![Figure 2.1 Electron scattering on single layer materials](image)

We start with a Point source electron beam impinging on a target consisting of a resist (PMMA) film. Figure 2.2 shows a sequence of events for one electron. In this simulation we take the Z axis as the direction of depth and the X-Y plane as the specimen surface.
When an electron of energy $E_0$ impinges in the material, the first scattering event, assumed to be at the surface, takes place. It involves the change in the angles $\theta$ and $\phi$. These are calculated from the differential cross section for elastic scattering cross section given by the Screen Rutherford's formula. The angle $\theta$ is chosen via a random number such that there is an equal probability for the integral of the elastic scattering cross section over the interval $(0, \theta)$. The azimuthal angle $\phi$ is chosen with uniformly distributed random number.

In a compound target, another random number is used to determine which atomic species serves as a scattering center. The probability for scattering by a particular atom is determined by the relative cross sections of the atoms that comprise the target. For each electron, a new set of random numbers is used, thereby ensuring that no two trajectories are identical.

The mean free path, which expresses the distance between two successive collisions, between elastic scattering events $\lambda$ is determined by the total elastic cross section. The first step takes a straight line without scattering because the first scattering event occurs after a finite penetration depth. Therefore, both values of $(\theta, \phi)$ have to be set to zero.

![Schematic showing the beginning of a typical electron for the Single scattering Model](image)
at the first step. Again, position $l$ (in fig. 2.2) of the electron after an elastic scattering at position $0$ is uniquely determined by $\theta$, $\phi$ and $\lambda$. The energy loss is calculated by Bethe's continuous slowing down approximation (CSDA). The calculation is repeated to yield new positions in the target for a new set of random numbers until the energy of the electron falls below a predefined value (500eV). The present calculation is performed up to 100,000 trajectories for a particular simulation. The important models for (1) electron scattering, (2) step length (mean free path) (3) scattering angles and (4) energy loss required in the simulation are described in the following.

2.3.1 Electron Scattering:

The differential scattering cross section when an electron interacts with a nucleus of an atom is given by the classical Rutherford equation. When electrostatic screening by shell electrons is taken into consideration, the Schrödinger equation has to be solved using an atomic potential. The solution with an exponential field based on the Born Approximation yields the following expression:

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{Z(Z+1)e^4}{4E^2(1 - \cos \theta + 2\beta)^2}$$

(2.12)

the term $Z(Z+1)$ is substituted for $Z^2$ in the classical theory to take account of the cross section for electron-electron collisions by simply assuming the same equation as that for electron-nucleus scattering.

The total cross section is obtained by integrating the above equation over the range of $\theta = 0, \pi$.

$$\sigma(\theta) = \int_{0}^{\pi} \frac{Z(Z+1)e^4}{4E^2(1 - \cos \theta + 2\beta)^2} d\Omega$$

(2.13)

where $Z$ is the atomic number, $e$ the electron charge, $E$ is the incident electron energy, $\theta$ the scattering angle and $\beta$ the screening parameter to account for electrostatic screening of the nucleus by the orbital electrons. The screening parameter $\beta$ is derived from the Thomas-Fermi model [98] for the atomic field, which is depend on the atomic potential utilized, and it is given by

$$\beta = \frac{1}{4} \left( 1.12 \frac{\hbar^2}{p} \right)^2 , \quad \lambda_0 = \frac{Z^{1/3}}{0.885a_0}$$

(2.14)
where \( \lambda_0 \) is Bohr radius, \( h \) is Planck's constant and \( p \) is the electron momentum. The value 1.12 is an adjustable parameter. The scattering parameter \( \beta \) is introduced in equation (2.14) to keep the total cross section constant.

Using the value of \( \sigma \), the mean free path \( \lambda \), is given by

\[
\lambda = \frac{A}{N_A \rho \sigma} = \frac{4E^2 A\beta(\beta + 1)}{\pi N_A \rho Z(Z+1)e^4} \tag{2.15}
\]

where \( N_A \) = Avogadro's no(atoms/mole), \( \rho \) = density(gm/cm\(^3\)), \( A \) = atomic weight (gm/mole) and \( \beta \) is the screening parameter.

Typically, an expression where \( \beta \propto (Z^{1/3}/E) \) is used, and very small values of \( \beta \) are encountered at the beginning of an electron trajectory. As the electron decelerates and \( E \) decreases, then \( \beta \) increases. However, since \( \beta \ll 1 \), it can be seen that \( \sigma \propto (1/E) \) and hence, \( \lambda \propto E \) (approximately). Thus in this single scattering model, the step length gets progressively smaller along the electron trajectory, and the total number of steps per trajectory can be very large.

### 2.3.2 Scattering Angles:

The scattering angle, directional cosine \( \cos(\theta) \) for a particular scattering event is chosen by means of Monte Carlo techniques by generating a uniformly distributed random numbers between 0 and 1. The probability \( P(\theta)d\Omega \) for scattering into a small solid angle \( d\Omega(=\sin \theta d\theta d\phi) \) is given by

\[
P(\theta)d\Omega = \left(\frac{d\sigma/d\Omega}{\sigma}\right)d\Omega \tag{2.16}
\]

The zenith angle \( \Phi \) is distributed uniformly from 0 to \( 2\pi \). Therefore Eq.(2.16) is only a function of \( \theta \). To evaluate the scattering angle \( \theta \) according to the probability \( P(\theta) \) we integrate Eq.(2.16) from 0 to \( \theta \) (using the definition of Eq. (2.13)) and obtain the following equation

\[
\theta = \cos^{-1}\left\{1 - \left[ \frac{2\beta F(\theta)}{1+\beta - F(\theta)} \right]\right\} \tag{2.17}
\]
where $F(\theta)$ is the accumulated function of $P(\theta)$. It can be easily shown that the angle $\theta$ is distributed in accordance with $P(\theta)$ when $F(\theta)$ is substituted by a uniform random number $R_1$. The atom specie which scatters the electron in a mixed target is also chosen by another random number, and is based on its fractional cross-section will be explaining in the following subsections.

Again the azimuthal angle $\phi$ can also be determined by generating another random number $R_2$ that is given by

$$\phi = 2\pi R_2 \quad (2.18)$$

### 2.3.3 Step Length:

We suppose that the step length, $s$, of a scattering electron between two successive collision events obeys to the Possion stochastic process with the probability distribution

$$P(s) = \lambda^{-1}e^{-s/\lambda} \quad (2.19)$$

where $\lambda$ is the elastic mean free path through

$$\lambda^{-1} \equiv \left( \int_0^\infty P(s)ds \right)^{-1} \quad (2.20)$$

By using an uniform random number, $R \in [0, 1]$, we can realize a value of $s$,

$$R = \int_0^s P(s')ds' = 1 - e^{-s/\lambda} \quad (2.21)$$

and hence,

$$s = -\lambda \ln(1 - R) \equiv -\lambda \ln(R) \quad (2.22)$$

### 2.3.4 Energy Loss:

Since the electron suffers scattering along its path, it continuously looses its kinetic energy along its path. This energy loss process of the electron when it traverses in the solid is a complicated process. The reason is that when the electron enters the solid it sees an assembly of atoms distributed in discrete and random fashion and the interaction of the electron with these atoms is quite complex. Therefore calculation of energy loss due to this complicated process is almost impossible. Hence Monte Carlo simulation with
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Bethe's continuous slowing down approximation is a nice empirical method of calculating this energy loss in electron-solid interaction. The mean energy loss along the trajectory between elastic scattering events to travel a path length $s$ along the trajectory is assumed to be given by the Continuous-slowing-down approximation of Bethe,

$$\Delta E = \int_0^s -\left(\frac{dE}{dx}\right) dx$$

where $-\left(\frac{dE}{dx}\right)_{\text{Bethe}} = 2\pi e^4 N_x \frac{1}{A \rho} \ln \frac{1.166E}{J}$

where $J$ is the mean ionization energy and the following empirical formula derived by Bulgers and Seltzers [99] is used for its derivation:

$$\frac{J}{Z} = 9.76 + 58.8Z^{-1.19}$$

The value of $J/Z$ is not constant but varies with $Z$, especially for low values of $Z$. Fortunately, this uncertainty in the numerical value of $J$ enters into the Monte Carlo simulation via a logarithm term and hence the sensitivity of the final result to this uncertainty is reduced accordingly.

We have finished the description of a randomly occurred scattering event. Let us describe the generalized position of the scattering events. Let $P(X_n, Y_n, Z_n)$ be the $n$th step the position of the scattering point then $P(X_{n+1}, Y_{n+1}, Z_{n+1})$, the $(n+1)$th step can be obtained as follows. The direction of electron motion $(\Theta_{n+1}, \Phi_{n+1})$ at the $(n+1)$th step in the $(x, y, z)$ coordinates is calculated by using the Euler equation:

$$\cos \Theta_{n+1} = \cos \Theta_{n} \cos \theta - \sin \Theta_{n} \sin \theta \cos \phi$$

$$\sin \Phi_{n+1} = U \sin \phi_{n} + V \cos \phi_{n}$$

$$\cos \Phi_{n+1} = U \cos \phi_{n} - V \sin \phi_{n}$$

where

$$U = \frac{\cos \theta - \cos \phi_{n} \cos \theta_{n-1}}{\sin \Theta_{n} \sin \Theta_{n+1}}$$
\[ V = \frac{\sin \phi \sin \theta}{\sin \theta_{n+1}} \]  

(2.29)

Thus, the position \( P_{n+1} \) is calculated as follows, using the step length \( s \) (from Eqn 2.22):

\[ x_{n+1} = x_n + s \sin \theta_{n+1} \cos \phi_{n+1} \]  

(2.30)

\[ y_{n+1} = y_n + s \sin \theta_{n+1} \sin \phi_{n+1} \]  

(2.31)

\[ z_{n+1} = z_n + s \cos \theta_{n+1} \]  

(2.32)

Tracing back the procedures described by Eqs. (2.12) – (2.32), we can then derive the second scattering position, and repeating this process forms an electron trajectory which is terminated only after either the electron having escaped from the surface or being rested in the sample (for a bulk sample there is no penetrating case) when its kinetic energy becomes below a cut-off energy, \( E \).

2.3.5 Parameters used in our simulation:

<table>
<thead>
<tr>
<th>Material Used</th>
<th>Average Density (( \rho )) gm/cm(^3)</th>
<th>Average Atomic Wt (A)</th>
<th>Ionization energy (eV)</th>
<th>Atomic Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMMA (C(_5)H(_8)O(_2))</td>
<td>1.23</td>
<td>100.067</td>
<td>( J_H = 18.7 ) ( J_C = 78.0 ) ( J_O = 89.0 )</td>
<td>( Z_H = 1.0 ) ( Z_C = 6.0 ) ( Z_O = 8.0 )</td>
</tr>
<tr>
<td>GaAs</td>
<td>((5.91+5.78)/2 = 5.845)</td>
<td>((69.717+74.922)/2 = 144.639)</td>
<td>Calculated from equation (2.24)</td>
<td>( Z_{Ga} = 31 ) ( Z_{As} = 33 )</td>
</tr>
<tr>
<td>Si</td>
<td>2.33</td>
<td>28.08</td>
<td>Calculated from equation (2.24)</td>
<td>( Z_{Si} = 14 )</td>
</tr>
<tr>
<td>SiC</td>
<td>2.475</td>
<td>40.09</td>
<td>Calculated from equation (2.24)</td>
<td>( Z_{Si} = 14 ) ( Z_C = 6.0 )</td>
</tr>
</tbody>
</table>
One characteristic feature of Monte Carlo calculations is the ease of setting geometrical boundary conditions just by changing input data such as incidence angle, or by programming a special specimen geometry. In electron beam lithography we can encounter various types of geometry depending on fabrication process technologies. One of the most important geometries is that of a thin resist film on a thick substrate. In the single layer simulation explained above, we calculate the mean free path using a random number only by the scattering probability appropriate to the layer which involves the initial scattering point. Therefore, when electrons are scattered from one certain layer to another layer, the calculated free path differs from an actual free path. Especially for multiple layers, which have very different scattering probability, the difference is expected to be large and cause errors in various simulation results.

Figure 2.3 shows the sequence of events of input an electron when the target is composed of a thin film (of PMMA) on top of a thick substrate (of GaAs or Si). A problem is how to handle electron transport behavior when electrons cross the boundary. The first approximation is to use the physical quantities at the starting point of the step to calculate the mean free path and scattering angle. When the initial step position comes close to an interface, the accuracy of this approximation becomes worse. Or in the case that there is
a large difference between the mean free paths on both sides of the interface, larger errors are induced. As the electron traverses the film-substrate boundary, parameters such as Atomic numbers, Z and ionization energy, J must be changed to describe the appropriate scattering and energy loss. The path of the electron will be changed due to the change in the properties of the second layer. Similarly when the electron happens to be backscattered again from the second layer to the first one, these changes will take place. In addition to the various fluxes of electron scattering, as shown by the paths a-f in figure 2.3, must be accounted for. When the electron crosses a boundary, the scattering and energy loss parameters appropriate to the initial point are used to calculate $\theta$, $\lambda$, and $\phi$. However, the parameters to the terminal point are used in the next calculations.

In our theoretical simulations we considered three substrates: Silicon, GaAs and SiC. The thickness of the resist film, PMMA is fixed at 1 $\mu$m. However its thickness can be varied to any depth. Electron beam energies starts from 20 keV to 100 keV. Thus, comprehensive range of practical electron lithography parameters has been considered and interpolation and extrapolation from our results is possible. Most of the models we used in single layers (Eqns. 2.12 to 2.32) are applied here. But for multiple layers, when electrons are scattered from one certain layer to another layer, the calculated free path differs from an actual free path. A technique is presented here for computing the distance between collisions as an electron is scattered from one layer to another where the scattering probabilities per unit length are different.

First the differential equation is introduced for the probability $P_m(s)$ that electrons once scattered at $z = 0$ are not scattered until $z=s$ in the $m$th layer is given by

$$dP_m(\Delta s) = -\sigma P_m(\Delta s)d(\Delta s)$$

(2.33)

where $P_1(\Delta s = 0) = 1, P_{m+1}(\Delta s = a_m) = P_m(\Delta s = a_m)$ and $a_m$ is the maximum depth in the $m$th layer. The solution of Eq. (2.33) gives the following probability $P_m(\Delta s)$ for the distribution of the variable step length:

$$P_m(\Delta s) = \frac{1}{\lambda_1} \exp \left( -\frac{\Delta s}{\lambda_1} \right), \text{ for } 0 \leq \Delta s \leq a_1$$

$$= \frac{1}{\lambda_m} \exp \left[ -\sum_{k=2}^{m} \left( \frac{1}{\lambda_{k-1}} - \frac{1}{\lambda_k} \right) a_{k-1} - \frac{1}{\lambda_m} \Delta s \right].$$
for $a_{m-1} < \Delta s \leq a_m, \quad m = 2, 3, ..., n$
\[= 0, \quad \text{for } a_m < \Delta s\] (2.34)

The accumulated function of $P_m(\Delta s)$ is used to determine the variable length $\Delta s$ in the usual manner as shown in single layer model Eq. (2.20).

According to this model, the mean free path for scattering depends on the initial position of the electron. Let us take an example of a PMMA resist film on a Si substrate. A mean free path $\lambda_p$ can be calculated as follows for an electron at a distance $x$ from the interface:

$$\lambda_p = \int_0^x sP_1(s)\,ds + \int_x^\infty sP_2(s)\,ds$$
$$= \lambda_{PMMA} - (\lambda_{PMMA} - \lambda_S)\exp(-x/\lambda_{PMMA})$$ (2.35)

where, $P_1$ and $P_2$ are the Probabilities per unit length of the first layer and second layer respectively. $s$ is the conventional free path and is given by

$$s = -\left(\frac{1}{W_1}\right)\ln R \quad \text{where } R = \text{Random no.}$$ (2.36)

The equation reduces to

$$\lambda_p = \lambda_S, \quad \text{for } x = 0$$
$$= \lambda_{PMMA} \quad \text{for } x = \infty$$ (2.37)

In this model, the mean free path $\lambda_p$ depends not only $\lambda_S$, but also $\lambda_{PMMA}$ and $x$, because the next layer along the scattering direction and the distance from the interface are taken into account.