Chapter -2

Experimental &
theoretical techniques

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2.1 Introduction

This chapter gives the basic principle of HPGe detector used in the present work. The instrumentation of a gamma ray spectrometry system has been briefly described. The spectrum analysis with reference to PHAST software has been discussed. Then, the basic principle and components of an input file of MCNP code used in the present work has been described.

2.2 Gamma ray Spectrometry with HPGe Detector

2.2.1 Basic Principle of Semiconductor Detector

Every solid material has its own characteristic electronic energy band structure. Highest occupied electronic energy band is called valence band and above which empty band exist called as conduction band. The energy gap between valence band and conduction band is called as band gap.

![Energy band diagrams of (a) Metal, (b) Insulator and (c) Semiconductor.](image)

**Figure 2.1** Energy band diagrams of (a) Metal, (b) Insulator and (c) Semiconductor.
Depending upon band gap, materials are classified as metal, insulator and semiconductor as shown in Figure 2.1. In case of metal, band gap is zero i.e. valence band and conduction band are overlapping [see Figure 2.1(a)]. Consequently under applied bias, electron can move with low resistance in conduction band. Whereas for insulator, a filled valence band containing no allowed empty state is separated from empty conduction band by band gap of about 4-5 eV, so no empty state is available to carry current under bias [see Figure 2.1(b)]. There are solid materials like silicon, germanium with band gaps in the range of 1 eV [see Figure 2.1(c)]. These types of materials are called semiconductors. Band gap of the semiconductor material is such that a few electrons can get thermally excited from valence band to conduction band leaving hole or positive charge in the valence band. These generated charge carriers (hole and electrons) carry small current under bias. Therefore current in semiconductor can be increased by increasing concentration of either holes or electrons. This has been achieved by doping the semiconductor material. Such doping add a new energy level in the band structure (see Figure 2.2).

**Figure 2.2** Energy level diagram of a p-type and n-type semiconductor.
To increase the hole concentration, the semiconductor crystal (e.g. Si/Ge) is generally doped with atoms with three valence electrons such as B, Al, Ga and In. This type of dopant introduces an impurity level near the valence band. These levels are close enough to accept electrons from valence band due to thermal excitation, leaving behind holes in the valence band. Since they accept electrons, the levels are called as acceptor levels and the semiconductor is called as p-type semiconductor. Similarly, to increase the electron concentration, semiconductor is doped with atoms having five valence electrons (e.g. P, As, Sb). This type of dopant introduces an impurity level near the conduction band. These levels are close enough to donate the electrons to conduction band due to thermal excitation, increasing the electron concentration in the conduction band. Since they donate electrons, the levels are called as donor levels and the semiconductor is called as n-type semiconductor.

When n-type and p-type semiconductor are joined together, electron moves from n-type region to p-type region and hole from p-type to n-type until an electric field is developed between the junction to oppose further accumulation of charge. Due to this charge carrier movement, a charge free region is created called as depletion region as shown in the Figure 2.3(a). Such p-n junction called as junction diode readily conducts electricity under forward bias (p-end is positively biased and n-end is negatively biased as shown in Figure 2.3(b) and the depletion region shrinks. In reverse bias, p-end is negatively biased and n-end is positively biased as shown in Figure 2.3(c), due to which depletion region increases and less current flows.
In solid state radiation detectors, when radiation passes, equal numbers of electron-hole pairs are created along its track (Figure 2.4). The generated charge is collected by applying an electric field which produces a voltage pulse. When forward biased, even in the absence of ionizing radiation, large current will flow across the semiconductor due to

Figure 2.3 Junction diode at (a) Zero bias (b) Forward bias (c) Reverse bias.
thermal excitation. This current will obscure the small current due to ionizing radiation. Whereas in case of a reverse biased junction, the current flowing through the semiconductor is negligible and the ionization current can be detected. Moreover, the sensitive volume of the detector i.e. the thickness of the depletion region is more, so that the semiconductors are generally reverse biased to be used as radiation detectors.

![Figure 2.4 Creation of electron-hole pair by interaction of radiation.](image)

In the case of a silicon or germanium of normal purity, the maximum depletion depth \( d \) beyond 2-3 mm (according to equation 2.1) is difficult to achieve even at breakdown voltage.

\[
d = \left( \frac{2eV}{
}\epsilon
N \right)^{1/2}
\]

(2.1)

where \( V \) is the reverse bias voltage, \( N \) is the impurity (dopant) concentration, \( \epsilon \) is the dielectric constant and \( e \) is the electronic charge. Gamma ray being highly penetrating in nature requires high depletion depth for detection. According to equation 2.1 for a given voltage, depletion depth \( (d) \) can be increased by reducing impurity concentration.
Techniques have been developed to manufacture high purity germanium crystal with depletion depths up to several centimeters. But for Si, manufacturing of such high purity crystal is not possible. The detector based on high purity Ge is known as high purity germanium (HPGe) detector. HPGe has low band gap of 0.67 eV at 300 K. So it can generate current (called leakage current) at room temperature. Therefore HPGe detector is operated at 77 K.

### 2.2.2 Configurations of HPGe Detector

Based on the shape of detector crystals, there can be two configurations of HPGe detector: planar and co-axial. Co-axial detectors can be open ended or closed ended, as shown in Figure 2.5. Co-axial detectors have large sensitive volumes (750 cc as compared to 10-30 cc of planar detectors) and therefore higher detection efficiencies than planar detectors. Although smaller in size, the planar detectors have best energy resolution because of their low capacitance and are generally preferred for low energy applications eg. for low energy gamma and X-ray spectra of uranium and plutonium.

![Figure 2.5 Different shapes of co-axial HPGe detectors](image-url)

(a) True co-axial (b) Closed-end co-axial (c) Closed-end co-axial (bulletized) [Knoll (2000)].
In co-axial HPGe detectors, two types of electrical contacts have been used: diffused contact is an $n^+$ layer and is the positive electrode and metal contact is a $p^+$ layer and is the negative electrode. These detectors can be generally classified as n-type and p-type detectors. In a p-type co-axial HPGe detector, the diffused contact is on the outside surfaces and the ion-implanted contact is given in the inner hole. Since the diffused contact is thicker, this limits the utility of the p-type detector for gamma rays below 40 keV. In contrast, an n-type co-axial detector, the thinner metal contact is on the outer surface and is usable down to 5 keV. Configurations of a p-type and an n-type closed end co-axial detector have been shown in Figure 2.6.

![Figure 2.6](image.png)

**Figure 2.6** Configurations of a (a) p-type and an (b) n-type closed-end co-axial detector [Knoll (2000)].

### 2.2.3 Characteristics of Gamma ray Spectra

A pulse height spectrum obtained at the end of the measurement reflects the energy deposition of the gamma ray in the detector as shown in Figure 2.7 for a $^{60}$Co source. It contains the contribution from all the three gamma ray interaction processes namely photoelectric absorption, Compton scattering and pair production.
Some of the important spectral features are:

(i) **Full energy peak:** Full energy peak is generated as a result of full energy deposition in the detector by photoelectric absorption, multiple Compton scattering or by deposition of full energy by the two 511 keV photons generated in the pair production as shown in the spectra (Figure 2.7) at 1173, 1332 and 2505 keV.

(ii) **Compton continuum:** This is generated due to partial energy deposition in the detector due to Compton scattering process.

(iii) **Compton edge:** The Compton edge appears at an energy corresponding to maximum energy loss by the gamma ray photon in a Compton scattering event. This corresponds to the Compton scattering interaction in which the gamma ray photon is backscattered and is labeled as CE corresponding to the Compton edges of gamma rays at energies i.e.1173, 1332 and 2505 keV respectively in the figure.
(iv) **Compton valley:** This corresponds to the partial energy deposition by a photon after undergoing multiple Compton events and lies between the Compton edge and the full energy peak.

(v) **Backscatter peak:** This arises due to Compton scattering of the gamma ray by more than $110^\circ$ in the surrounding material and generally occurs at 256 keV for a gamma ray of high energy. This is shown as BS in the Figure 2.7.

(vi) **Single escape peak:** This peak appears due to the escape of one 511 keV gamma ray produced in pair production and appears at $(E-511)$ keV as labeled in the Figure 2.7 as SE.

(vii) **Double escape peak:** This peak appears due to the escape of both the 511 keV gamma rays produced in pair production and appears at $(E-1022)$ keV as labeled in the Figure 2.7 as DE.

(viii) **Annihilation peak:** This is generated due to pair production of the scattered gamma ray in the surrounding material and subsequent annihilation of electron and positron formed, leading to generation of 511 keV gamma ray which is detected in the detector.

**2.2.4 Detector Parameters**

A detector is generally characterized by two parameters:

(I). **Resolution:** The resolution of the detector is the ability of the detector to resolve two nearby peaks. It is specified as Full Energy at Half Maximum (FWHM) given by:

$$FWHM = 2\sigma \sqrt{2\ln 2}$$

(2.2)
The % resolution \( R \) at a given energy \( E_0 \) is given by

\[
R = \frac{FWHM}{E_0} \times 100
\]  
(2.3)

Smaller is the \( R \), better is the resolution of the detector. For a co-axial HPGe detector, the value of \( R \) is very small and the resolution of detector is generally expressed in terms of FWHM at 1332 keV or at 122 keV for low energy.

(II). Detector Efficiency:

Absolute efficiency of a detector is defined as

\[
\varepsilon_{\text{tot}} = \frac{\text{total number of detected photons in the full energy peak}}{\text{total number of photons emitted by the source}}
\]  
(2.4)

This is the characteristic of the detector as well as the counting geometry and is expressed as the product of two terms:

\[
\varepsilon_{\text{abs}} = \varepsilon_{\text{geom}} \varepsilon_{\text{int}}
\]  
(2.5)

The geometric efficiency is given by

\[
\varepsilon_{\text{geom}} = \frac{\text{number of photons incident on the detector}}{\text{number of photons emitted by the source}}
\]  
(2.6)

This factor is independent of the gamma ray energy and depends upon the solid angle subtended by the source on the detector \( (\Omega) \) and is also written as:

\[
\varepsilon_{\text{geom}} = \frac{\Omega}{4\pi}
\]  
(2.7)

The geometric efficiency is responsible for the inverse square law of the variation of count rates as a function of source-to-detector distance.
The intrinsic efficiency is defined as

\[ \varepsilon_{\text{int}} = \frac{\text{number of pulses recorded}}{\text{number of photons incident on the detector}} \]  

(2.8)

This depends upon the detector characteristics i.e. on the atomic number \((Z)\) of the detector material. Assuming that the photon is normally incident on the detector, the intrinsic efficiency of a windowless detector can be given as:

\[ \varepsilon_{\text{int}} = 1 - e^{-\mu t} \]  

(2.9)

where \(\mu\) is the linear attenuation coefficient of the detector material and \(t\) is its thickness. Higher is the \(Z\), higher will be the intrinsic efficiency and higher will be the absolute efficiency of the detector. It is practically independent of the source-detector geometry.

Depending upon the nature of the events monitored, the absolute efficiency of the detector can be of two types:

(i) **Full energy peak efficiency**: Only the full energy peak is monitored where the counts may come due to full energy absorption of the gamma ray by any of the three interaction processes.

(ii) **Total efficiency**: All the events are monitored whether it leads to full or partial energy deposition.

The efficiency of an HPGe detector is generally specified by **relative efficiency** which means the efficiency of the detector at 1332 keV relative to efficiency for a point source at that energy of a 3” x 3” NaI(Tl) detector at a source-to-detector distance of 25 cm.
2.3 Instrumentation for Gamma ray Spectrometry

The electric signal produced as a result of collection of charge is analog in nature and is then processed in a pulse processing electronic chain. This typically consists of a preamplifier, amplifier, an analog-to-digital converter (ADC) and a multichannel analyzer (MCA) that produces the gamma spectrum. The components of a radiation detection system have been shown in Figure 2.8. The gamma spectrum is simply the number of photons detected in a preset number of channels, each channel corresponding to an energy band. Finally, the spectrum is analyzed in a PC using specialized software, performing energy and efficiency calibration, peak fitting, background subtraction, peak intensity calculation. The details of these components have been discussed in the following sections.

![Figure 2.8 Basic components of a radiation detection system.](image)

2.3.1 High Voltage Bias Supply

A bias voltage is required for collection of charge formed in the detector. This voltage is chosen high enough to ensure complete charge collection and low enough to avoid
voltage breakdown. In semiconductor detectors, bias supplies upto 5 kV are required. Electronic switching device, battery packs or charged capacitors can work as high voltage supplies.

2.3.2 Preamplifier

The preamplifier has two main functions: firstly, it converts the low amplitude, short duration current pulse from the detector into a voltage pulse whose amplitude is proportional to the energy deposited by the gamma ray in the detector. Secondly, it maximizes the signal to noise ratio of the output pulse and preserve the gamma ray energy information. To reduce the output noise level, the preamplifier is kept as close as possible to the detector. The output pulse from a preamplifier has a fast rise time (~ nanosecond) and a slow decay time (~ 50-100 µs).

2.3.3 Amplifier

The purpose of an amplifier is to amplify the pulses from the preamplifier into a linear voltage pulse in the range of 0 to 10 V. The amplifier also shapes the pulses to meet the requirements of the pulse height analysis instrumentation. This is important since the analyzer measures the input pulse amplitude relative to a reference voltage so that the output pulse from the amplifier should return as fast as possible to a stable voltage. This is vital for a high quality spectrum. Output pulses from the amplifier can be unipolar or bipolar. The former has a high signal to noise ratio leading to a better resolution. The latter, due to stable and easily detectable zero cross-over point, are used for timing applications.
2.3.4 Single Channel Analyzer

The pulse from the amplifier goes to a single channel analyzer which is a pulse height analysis instrument. Basically it contains two discriminators and only pulses with heights in between the two thresholds are allowed. It is connected to a scalar which will count the number of such pulses.

2.3.5 Multichannel analyzer

The multichannel analyzer (MCA) is the heart of most experimental measurements. It performs the essential functions of collecting the data, providing a visual monitor of the pulse height spectrum produced by the detector. An analog-to-digital converter (ADC) converts the analog voltage pulse from the amplifier into a binary output. The ADC sorts the pulses into a large number of channels according to the height of the voltage pulse and since the height is proportional to the energy of the gamma ray, the relationship between the channel number and energy is nearly linear. Two types of ADC’s are commonly used. They are called as Successive Approximation type ADC and Wilkinson type ADC.

2.4 Spectrum Analysis

Once the spectrum has been acquired it has to be analyzed to extract the desired information from the spectrum. Usually a gamma spectrum is used to give energy and number of photons emitted by the source [Debertin and Helmer (1988)]. Since the energy corresponding to full energy events is characteristic of a nuclide, though the spectrum contains all the events, usually only full energy events are monitored. After the
acquisition of spectra for the nuclide monitored, the peaks in the spectrum are analyzed with respect to their location (in channels), their peak area and full width at half maximum (FWHM). In this work, PHAST software [Mukhopadhaya, 2001] have been used for gamma ray spectrum analysis, therefore these operations have been discussed in the light of this software.

**Peak Location**

Although visual location of the peaks may be the best option, several methods [Mariscotti (1967), Black (1969), Conelly and Black (1970), Slavic and Bingulac (1970), Bullock and Large (1971), Lauterjung (1985)] have been developed to locate a peak in a spectrum. This becomes very useful when large number of peaks have to be located in the spectrum [Debertin and Helmer (1988)]. In PHAST, the derivative method developed by Mariscotti (1967) has been used. The peak shape is Gaussian in nature, which when differentiated two times i.e. when its second derivative is taken, gives a central large negative peak flanked by two smaller positive peaks. Whereas a smooth background gives, a constant first derivative and hence a zero second derivative and a Compton edge gives only one positive peak instead of two peaks as in a Gaussian peak. This behavior of the second derivative is considered as the signature of the peak and it is located at the centre of the negative lobe. If there are two or more closeby peaks than the behavior will be still different from a single peak.
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**Peak Area Determination**

Peak area is needed to get information about the number of photons of a particular energy detected in the detector. The peak area can be obtained by summing up the individual counts of all the channels under a peak. This method cannot be used for a complex spectrum where peaks may be overlapping with each other. Most ADC’s are equipped with peak area analysis softwares giving energy and intensity of peaks. Analytical fitting functions such as Gaussian functions are used in such softwares:

\[
f(x) = \frac{N}{w \sqrt{\pi / (4 \ln 2)}} e^{-\frac{(x-x_c)^2}{2\sigma^2}}
\]  

(2.12)

where \(N\) is the peak area, \(X\) is the centroid, FWHM, \(w = 2.35\sigma\). To analyze multiplets, the fitting function has to be modified by introducing additional Gaussian functions. Like for a doublet, the function will be given by:

\[
f(x) = \frac{N_1}{w_1 \sqrt{\pi / (4 \ln 2)}} e^{-\frac{(x-x_{1c})^2}{2\sigma^2}} + \frac{N_2}{w_2 \sqrt{\pi / (4 \ln 2)}} e^{-\frac{(x-x_{2c})^2}{2\sigma^2}}
\]  

(2.13)

So that, the number of unknown parameters increases to five: \(N_1, N_2, X_1, X_2\) and \(\sigma\). However, the actual gamma ray peak shape differs from the ideal Gaussian shape because of tailing on the low energy side. Several complex shape functions, taking the tailing into account, have been used in earlier well-known gamma analysis programs [Helmer and Lee (1980), McNelles and Campbell (1973)]. In PHAST software, a part of the Gaussian function is replaced by the exponential function [Routti and Prussin (1969)]:

\[
P(x) = \begin{cases} 
he^{-\frac{(x-p)^2}{2\sigma^2}}, & x \geq p-J \\
he^{-\frac{J(2x-2p+J)}{2\sigma^2}}, & x < p-J 
\end{cases}
\]  

(2.14)

The function is Gaussian for \(x \geq p-J\) and has a lower exponential tail smoothly joined at \(p-J\). A similar higher exponential tail may be used for peaks broadened by pile-up.
Moreover, since the full energy peaks rest on a background Compton continuum, this continuum must be subtracted from the gross peak area in order to get correct peak area. A large number of analytical functions representing this spectral background are available. Generally a linear function approximates the background sufficiently well unless there is a Compton edge in that region. In PHAST, a polynomial background function is used to represent the background.

\[ B(x) = a_0 + a_1 x + a_2 x^2 \]  

(2.15)

So the function fitted to a group of \( L \) peaks is

\[ F(x) = B(x) + \sum_{l=1}^{L} P_l(x) \]  

(2.16)

Also an option for addition of a step component corresponding to each peak is added to the background function to account for the escape of electrons from the sensitive volume of the detector giving rise to a step increase in count downwards from the photopeak energy. An option for selecting such terms is provided in the algorithm. The step increase below a peak at \( p \) is proportional to \( h \) and described in the program by the following function which takes into account the broadening of the step by the detector resolution function.

\[ S(x) = \alpha h \text{erfc}\left[\frac{x-p}{20.5 \sigma}\right] \]  

(2.17)

where \( \text{erfc}(x) \) is the complementary error function.

When this option is used, the function fitted to a group of \( L \) peaks is

\[ F(x) = B(x) + \sum_{l} S_l(x) + \sum_{l} P_l(x) , \text{ l=1 to L} \]  

(2.18)
**Peak Fitting Procedure**

Fitting involves minimization of the weighted sum $\chi^2$ of the square of the deviations of the data from the function $F(x)$.

$$\chi^2 = \sum_i \frac{(Y_i - F(x_i))^2}{Y_i}$$

(2.19)

The summation is performed over all the $n$ data points in the range of the peak group being fitted.

**Energy Calibration**

The ADC sorts the pulses according to their heights into different channel numbers. The energy calibration relates the channel numbers to the energy deposited by the particle in the detector. The energy calibration of a good spectroscopy system is nearly linear and is given by: $E = mx + b$ where $E$ is the energy deposited in the detector, $x$ is the pulse amplitude, $m$ and $b$ is the slope and intercept respectively. If more number of energies are present then value of $m$ and $x$ can be obtained by least square fitting. This method will distribute the deviations between the actual and computed energies more uniformly and also will reduce the sensitivity of the results to the particular choice of peaks and their location in the spectrum. This is required for the identification of nuclides.

$$m = \frac{n\sum x_i E_i - \sum x_i \sum E_i}{\Delta}$$

(2.20)

$$b = \frac{\sum x_i^2 \sum E_i - \sum x_i \sum x_i E_i}{\Delta}$$

(2.21)

where $\Delta = n\sum x_i^2 - (\sum x_i)^2$

A linear energy calibration upto second place of decimal is usually adequate for NDA applications. In PHAST, a polynomial function is used:
Shape calibration

Before fitting the gamma rays peaks, it is first necessary to calibrate the peak shape. For this, several single peaks with less error in peak area are fitted to second degree polynomials given as:

\[ E(x) = a_1 + a_2 x + a_3 x^2 \]  
(2.22)

\[ w(x) = (\alpha + \beta x)^{1/2} \]  
(2.23)

where \( w(x) \) is the FWHM of the peak at \( x \) channel number and \( \alpha \) and \( \beta \) are the parameters to be determined for FWHM calibration. FWHM calibration is important for resolving multiple peaks.

Efficiency calibration and activity calculation

For conversion of the measured count rate to the disintegration rate (\( dps \)) of the radionuclide monitored, it is important to calibrate the system for efficiency. Several fitting functions are available [Willet (1970), Gray and Ahmed (1985), East (1971), McNelles and Campbell (1973), Cox and Manneback (1985), Sanchez-Reyes (1987), Jackel (1987)]. Often two functions are used, one for lower energy (upto 200 keV) and other for higher energy range (above 200 keV). Generally a fourth order polynomial function is sufficient to fit the whole energy range from 80 keV to 2 MeV, as given by:

\[ \log E_i = \sum_{j=0}^{4} a_j (\log E_i)^j \]  
(2.24)

PHAST needs selection of energies and strength of the standard source in Bq for efficiency calibration.
2.5 MCNP Code

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. It takes into account the transport of both primary source electrons as well as secondary electrons created by gamma ray interactions in the medium.

It has been developed and maintained by Los Alamos National Laboratory (LANL) and is undergoing continuous development at LANL and its newer versions are released periodically. In the present work, version 4C [Briesmeister (2000)] has been used though its version 5 has already been released. Version 4 of the MCNP code was released in 1990 and was the first UNIX version of the code.

MCNP code is made up of about 48,000 lines of FORTRAN and 1000 lines of C source coding, including comments. This code is having about 385 subroutines. There is only one source code, which is used for all systems. For neutron transport, all reactions given in a particular cross-section evaluation (such as ENDF/B-VI) are accounted. For photon transport, the code takes into account photoelectric absorption, with the possibility of K- and L-shell fluorescent emission or Auger electron, coherent and incoherent scattering and pair production with the emission of annihilation radiation, and bremsstrahlung. For electrons, a continuous slowing down model is used that includes positrons, K X-rays, and bremsstrahlung but does not include external or self-induced fields. The neutron energy regime is from $10^{-11}$ MeV to 20 MeV, and the photon and electron energy regimes are from 1 keV to 1000 MeV.

In MCNP, a particle (neutron, photon or an electron) is randomly generated in the source volume and the path of the particle is tracked from its point of origin in the source to the
point of its complete absorption in the detector or upto its point of escape from the
detector. Along the track of the particle, the distance between two interactions and the
type of interaction that a particle undergoes are taken care randomly by its mean free path
and the relative probabilities of the different interactions ultimately related to the cross-
sections of the processes in question. In this way a large number of particles are
generated and ultimate result is given as the average of all the successes. Depending on
the number of particles generated, the error can be as small as desired by the user, given
sufficient time to complete the calculation. For example, consider the case of a photon of
energy $E$ emitted from a source placed on the detector surface as shown in Figure 2.9.
Half of the photons emitted by the source will enter the detector at all possible angles
from 0 to $\pi$ with respect to the detector axis. The photons while traveling through the
detector may or may not interact with the detector material. Whether an interaction will
take place or not and the distance between two interactions will be governed by the mean
free path ($\lambda = 1/\mu$, where $\mu$ is the linear attenuation coefficient of the medium at $E$) of the
photon in the detector material. Moreover, whether the particle will interact by a
photoelectric absorption, Compton scattering or a pair production will depend upon the
relative cross-sections of the three processes. If photoelectric absorption takes place then
the particle will deposit its full energy in the detector in one event only and the particle
will be tracked upto that point. But if Compton scattering or pair production takes place,
then there is a probability of photon to escape from the detector. Then the particle will be
tracked to the point of its last interaction.
MCNP is a very versatile and powerful transport code, and can model virtually any kind of geometry imaginable. A great advantage of MCNP is that one can vary the geometry of an experimental set-up as many times as needed without having to physically reproduce each change in the laboratory. This saves considerable expense and time by preventing to build and calibrate intermediate designs along the way. Specific areas of application include, but are not limited to, radiation protection and dosimetry, radiation shielding, radiography, medical physics, nuclear criticality safety, detector design and analysis, nuclear oil well logging, accelerator target design, fission and fusion reactor design, decontamination and decommissioning. Also, the MCNP code is commonly used in support of the design and calibration of NDA systems to be used for different applications such as for nuclear material safeguards applications [Weber (2006)]. The simulation can be applied to a range of detectors (high purity germanium detector in the case of gamma spectrometry, $^{3}$He detectors in the case of neutron counting devices), used
with a variety of radioactive sources including containers holding nuclear materials and drums containing neutron- and gamma-emitting waste.

Implementation of a Monte Carlo computational code requires the preparation of an input file which depends upon the problem dealt with. The detail of the input file is given in the following section.

2.5.1 Structure of the MCNP Input File

In the first step, an input file has to be created that describes the geometry of the system in three dimensions, and gives the description of materials including their densities, the location and characteristics of the emitting source, the type of results desired (given in terms of tallies) and variance reduction techniques to be used to improve efficiency of calculations. The geometry of MCNP treats an arbitrary three-dimensional configuration in user defined Cartesian co-ordinate system.

The input file has the following general form:

```
Message Block {optional}
Blank line delimiter {optional}
One Line Problem Title Card
Cell Cards [Block 1]
Blank line delimiter
Surface Cards [Block 2]
Blank line delimiter
Data Cards [Block 3]
Blank line terminator {optional}
```

**Figure 2.10** General structure of a MCNP input file.
Some of the important points to remember while making an input file are:

(i) The units to be used while giving an input in MCNP are: length in cm, energy in MeV, atomic densities in units of atoms/barn-cm and mass densities in g/cm$^3$. The output is also obtained in these units.

(ii) Characters written after 80 columns in a line are not read by MCNP while executing a file.

(iii) If the number of characters is more than 80, then it can be continued to the next line by using an & sign.

(iv) MCNP is not case sensitive.

(v) Anything that follows the $ is interpreted as a comment.

(vi) Blank lines are used as delimiters and as an optional terminator.

In MCNP, geometry of the concerned problem is treated primarily in terms of regions or volumes bounded by first and second degree surfaces defined with the help of Boolean operators. Geometry of the system is defined by defining cells and surfaces. As seen from Figure 2.10, the input file can be divided into four cards:

(I) Title Card (II) Cell Card (III) Surface Card (IV) Data Card.

The cell and surface card combines to give the complete geometry specification of the problem, while the data card carries the information about materials and selection of cross-section evaluation. Source specification inputs and the required tally types are also given in the data card. Each card is separated by a blank line. These cards have been discussed in details in the following sections.
(I) Title Card

This card gives the title of the problem in one line. It can contain any information you desire but usually contain information describing the particular problem (or can even be blank). The first line in the input file is reserved for this card if there is no message block.

(II) Cell Card

A cell is a region bounded by the surfaces. The full geometry of the concerned problem is divided into a certain number of cells. Each cell is described by a cell number, material number, and material density followed by a list of signed surfaces that bound the cell. Cells are defined by intersections or unions of surfaces defined in the surface card. Intersection operator is simply the blank space while a union operator is defined by ‘:’ sign between the two surfaces. The union and the intersection operators can be understood by considering a pair of concentric circles (with surfaces defined as 1 and 2) as shown in Figure 2.11.

Figure 2.11 Intersection (a) and union (b) of two surfaces 1 & 2.
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The region that belongs to both 1 and 2 is called the intersection of 1 and 2 (i.e. \( 1 \cap 2 \), shown as the lined area in Figure 2.11(a). The region containing points that belong to 1 alone or to 2 alone or to both 1 and 2 is called the union of 1 and 2 (i.e. \( 1 \cup 2 \), shown as the lined area in the Figure 2.11(b). Unions and intersections of geometric surfaces can be used in a combined way to define a cell. Note that a parenthesis is equivalent to a space and signifies an intersection. Apart from this one more Boolean operator is used i.e. NOT denoted by ‘#’. It acts as a complementary operator. For example \# (1:2) represents all space outside the union of 1 and 2. If a cell is defined by only intersections, then all the points within a cell should have same sense (either +ve or –ve) with respect to a given bounding surface. A cell card consists of the cell number, material number, and material density in sequential way separated by spaces, followed by a complete specification of the geometry of the cell. The cell number must begin in columns 1–5. The specification includes a list of signed surfaces bounding the cell where the sign denotes the sense of the regions defined by the surfaces. A void cell (e.g. universe) is defined by giving the material number and material density by a zero. The blank line terminates the cell card of the input file. It is always better to define a large number of simple cells rather than defining few complicated cells.

Form of a cell card: \[ \text{cn mn md geom params} \]

\begin{align*}
\text{cn} &= \text{cell number}. \\
\text{mn} &= \text{material number (0 if the cell is a void)}. \\
\text{md} &= \text{cell material density (absent if the cell is a void)}. 
\end{align*}
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geom = specification of the geometry of the cell. It consists of
signed surface numbers and Boolean operators that specify how the regions bounded by
the surfaces are to be combined.

params = optional specification of cell parameters by entries in the
keyword.

(III) Surface Card
A surface can be defined in two ways in MCNP: (1) by specifying known geometrical
points on a surface that is rotationally symmetric about a co-ordinate axis, or (2) by
supplying the appropriate coefficients needed to satisfy the surface equation. The former
method can be used only if one is setting up geometry from something like a blueprint
where one knows the co-ordinates of intersections of surfaces or points on the surfaces.
In the latter method, a surface is defined using one of the surface-type mnemonics as
given in Table 2.1 and calculating the appropriate coefficients needed to satisfy the
surface equation. In a surface card, the surface number, alphabetic mnemonic indicating
the surface type, numerical coefficients of the equation defining the surface are given in
the sequential order. The surface number must begin in columns 1-5 and not exceed 5
digits.

Form of a surface card:  sn  n  a  cf

\[ sn = \text{surface number} \]
\[ n = \text{required only when co-ordinate transformation is there.} \]
\[ a = \text{equation mnemonic from Table 2.1} \]
\[ cf = \text{list of coefficients of the equation describing the surface.} \]
### Table 2.1 Specifications of a surface in MCNP.

<table>
<thead>
<tr>
<th>Mnemonic*</th>
<th>Description</th>
<th>Equation</th>
<th>Card entries required</th>
</tr>
</thead>
<tbody>
<tr>
<td>P</td>
<td>General</td>
<td>( Ax + By + Cz - D = 0 )</td>
<td>ABCD</td>
</tr>
<tr>
<td>PX</td>
<td>Normal to x axis</td>
<td>( x - D = 0 )</td>
<td>D</td>
</tr>
<tr>
<td>PY</td>
<td>Normal to y axis</td>
<td>( y - D = 0 )</td>
<td>D</td>
</tr>
<tr>
<td>PZ</td>
<td>Normal to z axis</td>
<td>( z - D = 0 )</td>
<td>D</td>
</tr>
<tr>
<td>SO</td>
<td>Centered at origin</td>
<td>( x^2 + y^2 + z^2 - R^2 = 0 )</td>
<td>R</td>
</tr>
<tr>
<td>S</td>
<td>General</td>
<td>( (x - \bar{x})^2 + (y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0 )</td>
<td>( \bar{x} \bar{y} \bar{z} ) R</td>
</tr>
<tr>
<td>SX</td>
<td>Centered on x axis</td>
<td>( x^2 + (y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0 )</td>
<td>( \bar{x} ) R</td>
</tr>
<tr>
<td>SY</td>
<td>Centered on y axis</td>
<td>( (x - \bar{x})^2 + y^2 + (z - \bar{z})^2 - R^2 = 0 )</td>
<td>( \bar{y} ) R</td>
</tr>
<tr>
<td>SZ</td>
<td>Centered on z axis</td>
<td>( (x - \bar{x})^2 + (y - \bar{y})^2 + z^2 - R^2 = 0 )</td>
<td>( \bar{z} ) R</td>
</tr>
<tr>
<td>C/X</td>
<td>Parallel to x axis</td>
<td>( (y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0 )</td>
<td>( \bar{y} \bar{z} ) R</td>
</tr>
<tr>
<td>C/Y</td>
<td>Parallel to y axis</td>
<td>( (x - \bar{x})^2 + (z - \bar{z})^2 - R^2 = 0 )</td>
<td>( \bar{x} \bar{z} ) R</td>
</tr>
<tr>
<td>C/Z</td>
<td>Parallel to z axis</td>
<td>( (x - \bar{x})^2 + (y - \bar{y})^2 - R^2 = 0 )</td>
<td>( \bar{x} \bar{y} ) R</td>
</tr>
<tr>
<td>CX</td>
<td>On x axis</td>
<td>( y^2 + z^2 - R^2 = 0 )</td>
<td>R</td>
</tr>
<tr>
<td>CY</td>
<td>On y axis</td>
<td>( x^2 + z^2 - R^2 = 0 )</td>
<td>R</td>
</tr>
<tr>
<td>CZ</td>
<td>On z axis</td>
<td>( x^2 + y^2 - R^2 = 0 )</td>
<td>R</td>
</tr>
</tbody>
</table>

*P, S and C indicates the surface type to be plane, sphere and cylinder respectively
Every surface has a “positive” side and a “negative” side. A point \((x, y, z)\) is defined as having positive sense with respect to a surface when the expression for that surface evaluated at \((x, y, z)\) is positive and vice versa. For example, if a cylinder (with its axis along the x-axis) is a surface then from Table 2.1, the equation for the cylinder will be:

\[
y^2 + z^2 - R^2 = 0
\]  

(2.25)

This surface can be divided into two regions: one outside it and the other inside it. When a point \((x, y, z)\) lies outside the cylinder, then the LHS of the equation at \((x, y, z)\) will be positive, therefore the point \((x, y, z)\) will have a positive sense with respect to this surface and when this point lies inside the cylinder, the LHS of the equation at \((x, y, z)\) will be negative, therefore the point \((x, y, z)\) will have a negative sense with respect to this surface.

If this cylinder has a radius of 2.5 cm with its axis along x-axis and is the 3rd surface in the sequence then in the surface card it will appear as

\[
3 \text{ CX 2.5}
\]

(IV) Data Card

This card specifies the information about the source and the material involved in the problem. This card itself can be divided into a number of cards given below:

1. MODE Card

It gives the mode of transport of the particle in the study. It can be single transport mode like a neutron or a photon or an electron, or it may be coupled. Different transport modes and their corresponding mnemonics are given below.
\( N \) — neutron transport only
\( P \) — photon transport only
\( E \) — electron transport only
\( P E \) — photon and electron transport
\( N P \) — neutron and neutron induced photon transport
\( N P E \) — neutron, neutron induced photon and electron transport

If the MODE card is omitted, mode \( N \) is assumed.

2. Cell and Surface Parameter Cards

It includes the \( \text{IMP:} \) particle mnemonic (eg. \( N \) or \( P \)) card giving the relative cell and surface importances in the sample problem. It is represented as \( \text{IMP:\(N\)}, \text{IMP:\(P\)}, \text{IMP:\(N\) \(P\)}, \text{IMP:\(P\) \(E\)}, \text{IMP:\(N\) \(P\) \(E\)} \) etc.

For eg. \text{IMP:\(N\) 1}

This means that the neutron data (it can be flux, current etc.) in the cell 1 is the desired output.

3. Source Specification Cards

It is denoted as \( \text{SDEF} \) and gives the specifications of the source. Some of the parameters defined in this card are:

\( \text{POS} = x \ y \ z \) (default is 0 0 0);

\( \text{CEL} = \) starting cell number (not required for a point source);

\( \text{ERG} = \) starting energy (default is 14 MeV);
$WGT =$ starting weight (default is 1);

$TME =$ time (default is 0);

$PAR =$ source particle type 1 for N, N P, N P E; 2 for P, P E; 3 for E.

### 4. Tally Specification Cards

Since MCNP can be used for a variety of purposes, depending upon the type of output required (like current across a surface, flux at a point etc.), different tally cards are used. The different types of tally cards and their corresponding descriptions are given below.

<table>
<thead>
<tr>
<th>Tally type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F1$</td>
<td>Surface current</td>
</tr>
<tr>
<td>$F2$</td>
<td>Surface flux</td>
</tr>
<tr>
<td>$F4$</td>
<td>Track length estimate of cell flux</td>
</tr>
<tr>
<td>$F5$</td>
<td>Flux at a point or ring detector</td>
</tr>
<tr>
<td>$F6$</td>
<td>Track length estimate of energy deposition</td>
</tr>
<tr>
<td>$F7$</td>
<td>Track length estimate of fission energy deposition</td>
</tr>
<tr>
<td>$F8$</td>
<td>Energy distribution of pulses created in a detector</td>
</tr>
</tbody>
</table>

An $F8$ tally, known as a pulse height tally, was used in all models. This tally records the energy deposited in a cell by each source particle and its secondary particles. A Gaussian Energy Broadening ($GEB$) treatment was used to simulate the resolution of the detector. This treatment uses three parameters to define the resolution of the detector at a specific energy by:

$$FWHM = a + b\sqrt{E} + cE^2$$  \hspace{1cm} (2.26)
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\[ E = \text{the peak energy (MeV)}, \]

\[ FWHM = \text{the full width at half maximum of a Gaussian resolution function centered at } E, \]

\[ a, b, c = \text{parameters whose values are required as an input and are generally obtained by using the experimental } FWHM \text{ calibration curve.} \]

5. Materials Specification Card

This card gives the details of the materials i.e. the isotopes present and their fractions in a given material. The general format is

\[
\begin{align*}
\text{Mm} & \quad \text{ZAID}1 \quad \text{fraction}1 \\
\text{Mm+1} & \quad \text{ZAID}2 \quad \text{fraction}2
\end{align*}
\]

where \( m \) denotes the material number and the material is identified by the number \( ZAID \) with the form \( ZZZAAA.nnX \), where \( ZZZ \) and \( AAA \) gives the \( Z \) and \( A \) of the isotope. Conventionally, \( nn \) and \( X \) are the cross-section evaluation identifier; if blank or zero, a default cross-section evaluation will be used, and class of data respectively, \( C \) is continuous energy, \( D \) is discrete reaction, \( T \) is thermal, \( Y \) is dosimetry, \( P \) is photon, \( E \) is electron and \( M \) is multigroup. Fraction gives the fraction of the isotope present in the material.

A typical input file has been given in the Appendix I of this thesis.