JOINT INSTITUTE FOR NUCLEAR RESEARCH

Frank laboratory of neutron physics

FINAL REPORT ON THE START PROGRAMME

Simulation of semiconductor heterostructures under the influence of neutron radiation of various energies in the Geant4 environment

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CONTENT

1. Literature review

1.1. Semiconductors

It has been over four decades since the conceptualization of the high electron mobility transistor (HEMT) in 1979 [1]. The fundamental principle underlying the HEMT technology involves the field-effect modulation of a high-mobility two-dimensional electron gas (2DEG) within a heterostructure comprised of selectively doped semiconductor pairs, notably including n-AlGaAs/GaAs and n-InAlAs/InGaAs configurations. The initial experimental validation of the HEMT concept was achieved by research group in the year 1980 [2]. Subsequently, in the same period, documented the inaugural demonstration of superior microwave performance, surpassing that of a GaAs metal–semiconductor field-effect transistor (MESFET) [3]. The year 1981 marked a significant milestone with the development of the first HEMT digital integrated circuit, showcasing unprecedented switching speeds within the semiconductor landscape [4]. Following pioneering endeavors, a global initiative ensued to advance the capabilities of high-speed, high-frequency HEMTs.

In 1985, a pivotal advancement occurred as HEMTs found commercial application as cryogenic low-noise amplifiers, enhancing radio telescope sensitivity to detect microwave signals emanating from dark nebulae, leading to the serendipitous discovery of a novel interstellar molecule [5]. The mass production of HEMTs for consumer applications commenced circa 1986, where low-noise HEMT amplifiers were predominantly integrated into broadcasting satellite receivers, laying a robust technological foundation for subsequent advancements in microwave and millimeter-wave applications, including but not limited to cellular handset devices [6] and automotive radar systems [7].

The history of the development of the HEMT at laboratories began with research into GaAs metal–oxide–semiconductor field-effect transistors (MOSFETs) in 1977. The research was motivated by the expectation that GaAs MOSFETs would offer superior high-speed performance over Si-based counterparts.

Figure 1 shows a sketch depicting the device principle of HEMTs. The sketch illustrates how the energy band diagram of the system changes with the n-type AlGaAs layer thickness. When AlGaAs is thick, as in the leftmost drawing of Figure 1, there are three regions in the n-type AlGaAs layer; the surface depletion region formed by a Schottky barrier, a charge neutral region, and the interface depletion region at the heterojunction. In this configuration, we cannot fully control the electron accumulation layer because the charge neutral region effectively shields the electric field from the gate. Due to this limitation, successful HEMT operation is not possible. With AlGaAs of medium thickness, as in the middle of Fig. 1, the two depletion regions merge, the entire AlGaAs layer is depleted, and the electron accumulation layer remains at the interface. In this profile, the electric field from the gate reaches and modulates the electron accumu-lation layer at the interface. This results in depletion-mode HEMTs (called D-HEMTs). The first demonstration of D-HEMTs was published in May 1980 [2]. When the AlGaAs layer is thin, since the pinning point of the Fermi level on the AlGaAs surface is below the conduction band of the GaAs layer, the electron accumulation layer disappears, as shown in the rightmost drawing. When positive gate voltages higher than the threshold voltage are applied, an electron accumulation layer is induced at the interface. This explains the operation principle of enhancement-mode HEMTs (called E-HEMTs).

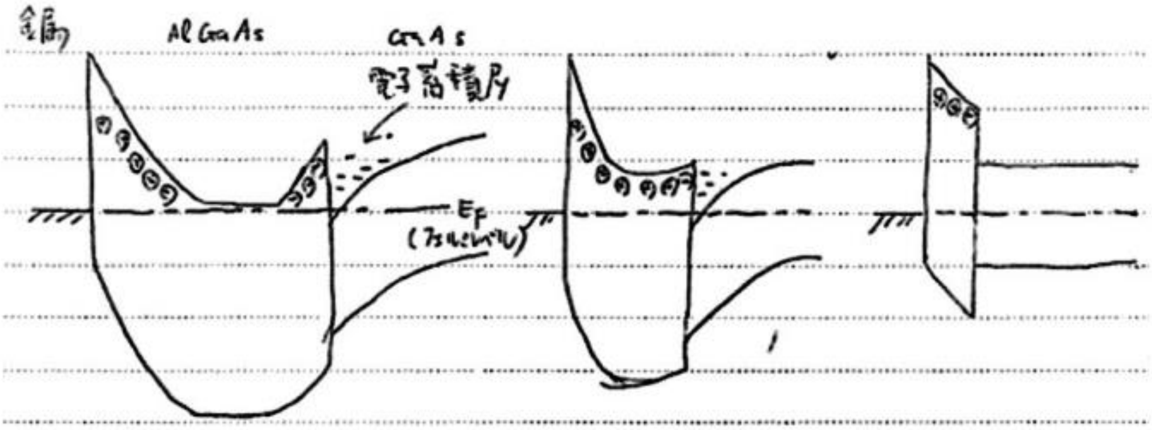


Figure 1.1 Energy band diagrams explaining field-effect modulation of two-dimensional electron gas.

The paragraph outlines the evolutionary trajectory of HEMT technology within the realm of digital integrated circuit (IC) applications. In 1981, a seminal milestone was reached with the unveiling of the first HEMT integrated circuit [4]. Figure 2 provides an intricate depiction of the HEMT ring oscillator, a conventional test circuit instrumental in gauging the switching performance of a fundamental logic gate.

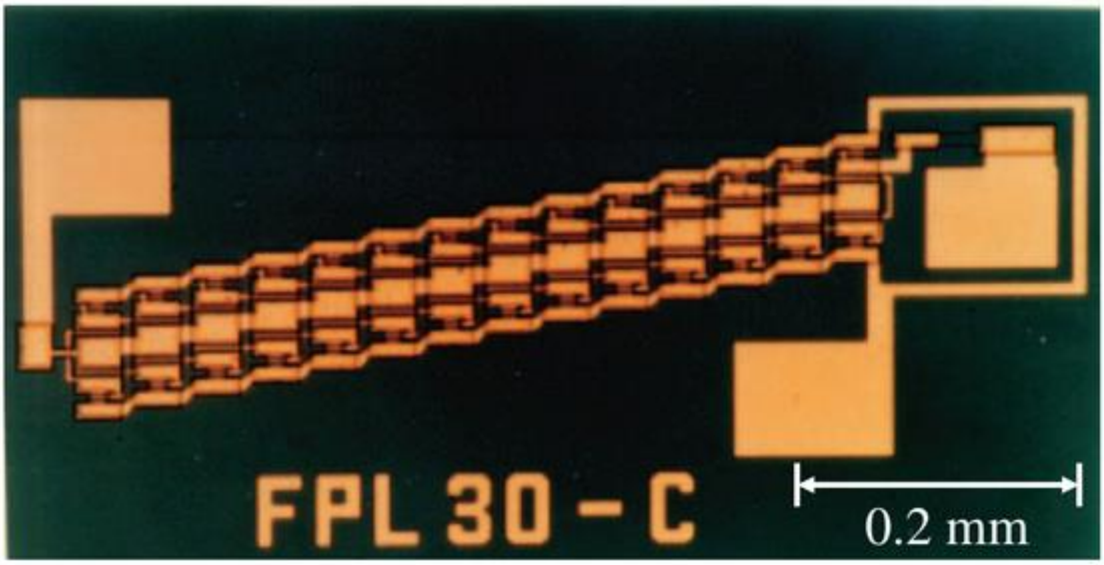


Figure 1.2 First HEMT integrated circuit: 27-stage ring oscillator.

Figure 3 offers an in-depth cross-section view of a typical HEMT direct-coupled FET logic (DCFL) circuit, comprising both E- and D-HEMTs. In this configuration, the gate metal of a D-HEMT is situated on a GaAs cap layer to establish a negative threshold voltage. A pivotal technological advancement facilitating the integration of E- and D-HEMTs within the same epitaxial wafer involved the utilization of selective dry etching to meticulously control the threshold voltage of E-HEMTs. Notably, the selective removal of the GaAs cap layer from the gate region of E-HEMTs via dry etching using CCl2F2 and He yielded a high selectivity ratio exceeding 260 [16]. This breakthrough in selective dry etching proved instrumental in the fabrication of LSI circuits, particularly for the mass production of recessed gate structures widely adopted in low-noise HEMTs.

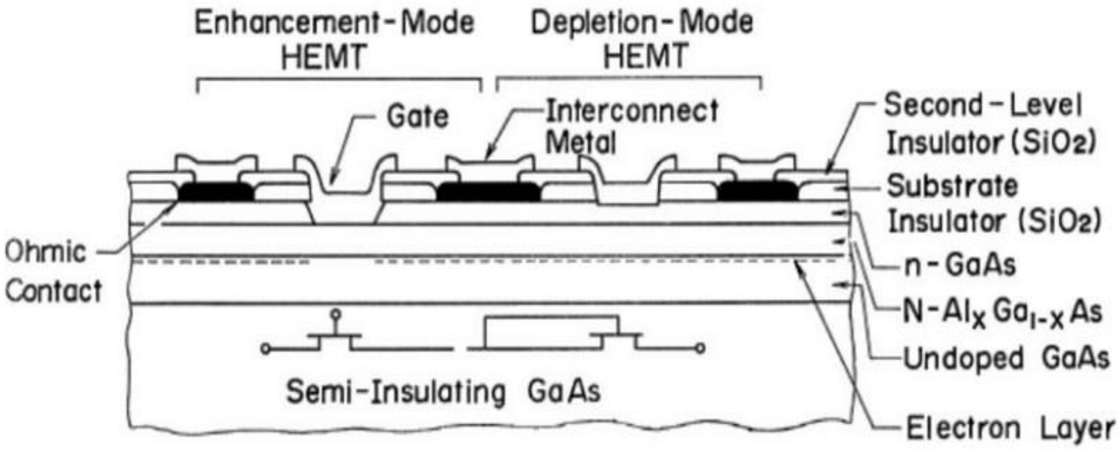


Fig. 1.3. Schematic cross section of logic gate consisting of E- and D-HEMTs.

Looking ahead, the miniaturization of HEMTs is anticipated to enhance their high-speed, high-frequency performance. Decreasing the horizontal dimensions of the device, such as gate length, necessitates a simultaneous reduction in vertical dimensions to mitigate the short-channel effect, adhering to the scaling rule for FETs. From a scaling perspective, InP emerges as a favorable alternative to GaAs due to its capacity for thinner barrier layers in InP-based HEMTs compared to their GaAs-based counterparts at equivalent threshold voltages and donor concentrations in the barrier layers. This advantage stems from the narrower energy differential between the Schottky barrier height of the gate and the conduction band offset at the heterointerface in InP-based devices relative to GaAs-based variants, typically ranging from 0.1 to 0.2 eV for InP and 0.4 to 0.5 eV for GaAs-based HEMTs.

The evolution of HEMTs since their inaugural demonstration in 1980 has been nothing short of remarkable. The pervasive availability of HEMTs, particularly in microwave and millimeter-wave applications, has transcended initial expectations. Future endeavors are poised to concentrate on device miniaturization, leveraging wide-band-gap III–V nitrides to bolster fundamental device performance, with a concerted effort towards achieving substantial cost efficiencies.

1.2. Radiation resistant semiconductors

Semiconductor based devices find many applications in harsh radiation environments such as space, for satellite optocouplers, and radiation physics laboratories, for particle detectors [13 - 14]. Serious damage due to the radiation effects such as increment in the leakage current [15 - 16] and reduction in the charge collection efficiency [17] may occur in such devices if proper shielding is not well integrated. However, to some devices such as sensors and radiation detectors, direct shielding may hinder the device‘s useful function which, at length, will result in precision and accuracy deterioration.

Since some heavy metals, such as copper and tungsten, are better conductors than aluminium, metal components for interconnection of semiconductor chips can be smaller in size with them, and consume less energy when electricity passes through them while keeping higher-performance. Therefore, in semiconductor integrated circuits, tungsten and copper are widely used. In complementary metal oxide semiconductors (CMOS), incident neutrons, protons, and heavy-ions can induce a single event upset (SEU) in its sensitive volume (SV). Here, we will focus on neutron induced single event upset. In silicon, secondary particles created by nuclear interactions of incident neutrons can range from H to Si, eventually P, including isotopes [18]. According to the primary neutron energy and the details of the interaction, all these particles have variable energies, linear energy transfers (LETs) and free paths. SEU is caused by the electrical changes associated with the electron-hole pairs generated along the ionising particle track. When the number of electron-hole pairs is more than the critical charge in the SV of the CMOS, an SEU will occur.

During the last decades, the magnetic field sensors and especially the Hall sensors (Hall-plate sensors, Hall effect transducers) attracted significant academic and industrial interest. The magnetic field sensors are the basis of many high technology products, such as apparatus for linear and angular displacements, position change, non-contact measurement of AC and DC current and electrical power, signal amplifiers in telecommunication, spatial detectors of metal objects, three-dimensional vector magnetometers, compasses, etc. [13, 14]. Here we will address the problems of radiation-resistant semiconductors technology for Hall magnetic sensors.

Semiconductors are divided into three groups based on electrical neutrality: The first group includes wide-gap materials like Si, GaAs, and AlAs, which exhibit equal electron and hole concentrations, characteristic of highly resistive, fully compensated semiconductors. The second group, with materials like InAs and InP, shows a much higher electron concentration than hole concentration, leading to n-type conductivity. The third group comprises semiconductors like Ge, InSb, GaSb, and AlSb, where the hole concentration surpasses the electron concentration, resulting in p-type conductivity after irradiation.

In high-energy particle irradiation, the radiation defects in semiconductors are accumulated in the crystalline lattice, which causes the change of the Fermi level position, which leads to considerable changes in the material’s electrophysical properties. The nature and properties of the radiation defects, especially in the compound semiconductor, are not known enough even nowadays, despite numerous investigations. Thus the development of the irradiation semiconductor’s model, which does not require detailed information about the nature and the parameters of the radiation defects, is effective for the quantitative evaluation of the electrophysical parameters of the irradiated semiconductor.

According to modern theoretical models and experimental investigation, the parameters of the irradiated semiconductor depend primarily on the intrinsic fundamental characteristics of the materials (e.g., energy-band structure) and somewhat on the conditions of irradiation and materials' prehistory. A range of investigations was performed for the experimental verification of the basic principle of irradiated semiconductor's theoretical model, which is a slight dependence of characteristics of the materials investigated InSb and InAs upon the prehistory of the materials, which is a method of obtaining and doping.

The performed investigation has shown that for both InAs and InSb the stability of characteristics at the testing in neutron fluxes depends on the value of charge carrier concentration only and does not depend on the material's prehistory, i.e., the method of growing and doping impurity introduction. Fig. 1 and Fig. 2 show the results of the test of InSb<Sn> and InAs<Sn> crystals irradiated in the neutron flux up to the fluence of $F = 1\cdot10^{15}$ n·cm−2 and obtained by the different methods. The obtained results are represented on the dependence curves of relative charge carrier concentration vs. initial concentration in crystals. These changes have the minimum values at the initial concentration for InSb of $n0 = (6 \div 7)\cdot10^{174}$ cm−3, and for InAs – $n0 = (2\div3)\cdot10^{18}$ cm-3, which are in good agreement with the results of the previous investigations for InSb and InAs microcrystals. Thus, the performed experimental investigations confirmed the principle of the theoretical model of irradiated semiconductors about the independence of InSb and InAs irradiated materials' properties of the materials' prehistory, which is the method of obtaining and crystal doping.

However, the difference in the quality of the obtained materials when comparing the methods of nuclear doping and metallurgical doping in the growing process with the following radiation modification is considerable. It is represented in the degradation of basic electrophysical properties of nuclear-doped samples compared to the samples doped metallurgically in the growing process. This difference is especially notable in structurally perfect microcrystals of InSb and InAs, obtained from the gas phase.

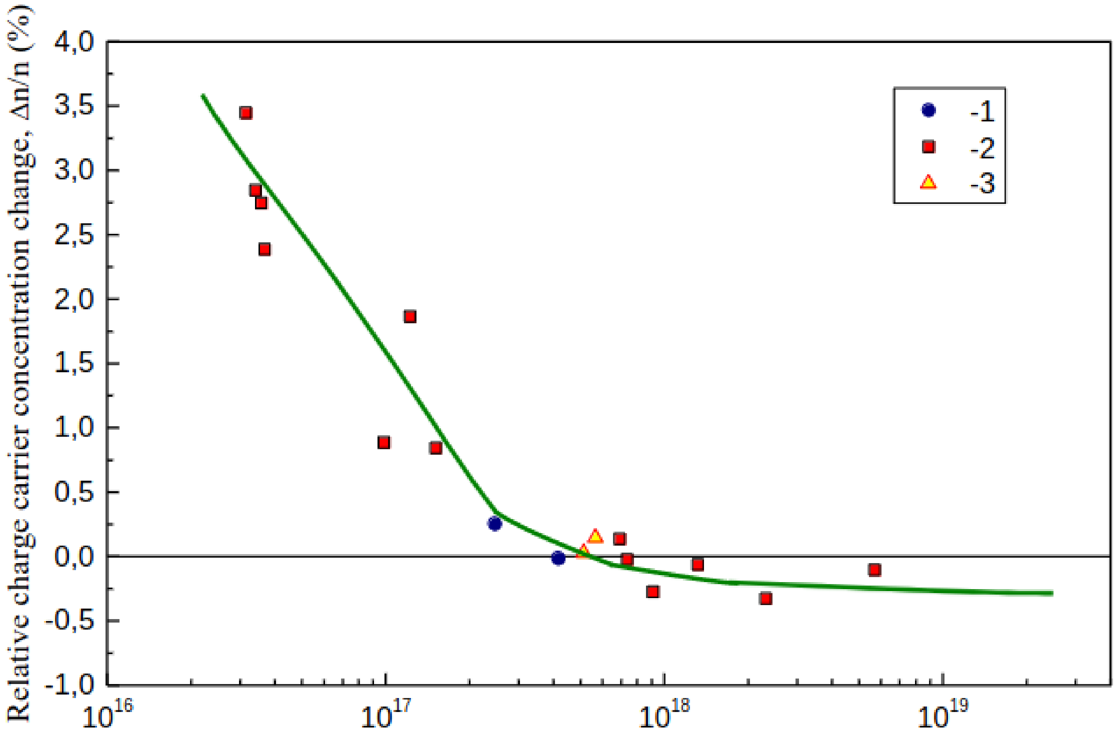


Figure. 1.4 Concentration dependence of relative change of charge carrier concentration for the samples of InSb<Sn>.

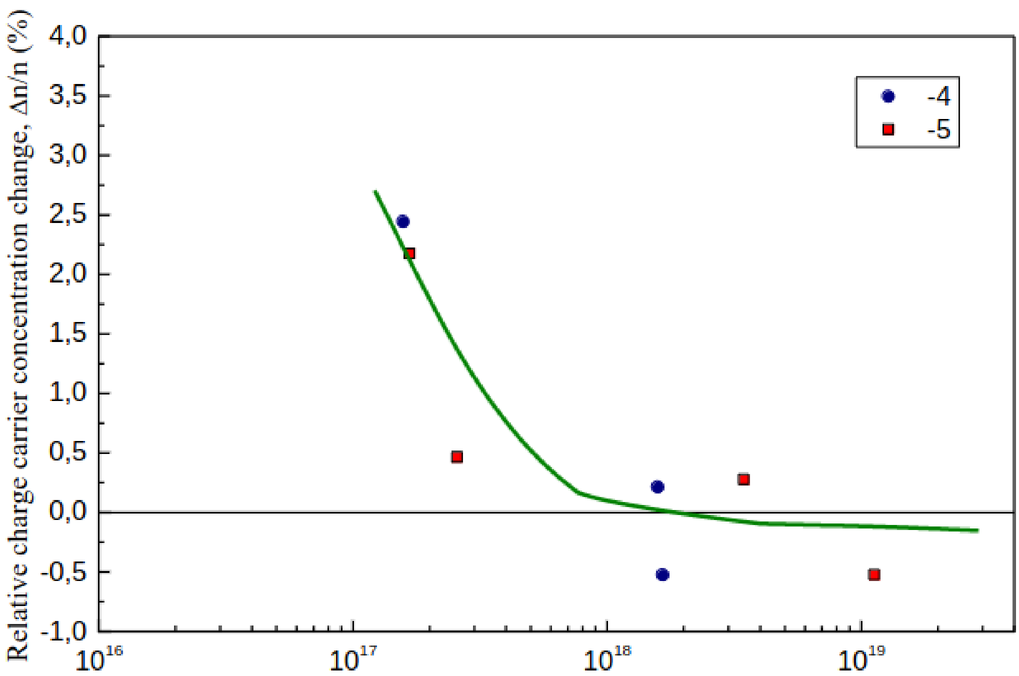


Figure. 1.5. Concentration dependence of relative change of charge carrier concentration for the samples of InAs<Sn>.

The technology of InSb, InAs and GaAs semiconductor microcrystals growth being doped by donor, isovalent, rare-earth impurities and based-on impurity complexes has been developed. The technology uses a CVD flow system. The shape of whiskers and thin films have a very high level of structure perfection. They are effective prototype samples for the investigation of radiation stability and prototyping magnetic field sensors.

Figure. 1.6 - Photographs of the microcrystals InSb , InAs , GaAs .

Researchers have been studying how different impurities affect the electrical properties of crystals. They found that by adding tin (Sn), a type of impurity, they could control the number of charge carriers (like electrons) in microcrystals of materials called InSb and InAs. The number of these charge carriers could be adjusted from 10^{15} to 10^{18} per cubic centimetre. When they added a rare earth element called ytterbium (Yb) to InSb, it resulted in fewer charge carriers but they moved faster, especially when interacting with the tin atoms already in the material.

Another discovery was that using a mix of impurities (Sn, Al, and Cr) increased the energy gap of the crystals by 22% compared to crystals without these impurities. This energy gap is important for the crystal's electronic properties. The researchers also found the best combination of these impurities to make the crystal's properties stable, even when exposed to radiation.

They developed a complex method to create very stable microcrystals of InAs and InSb, which are used in magnetic field sensors that can withstand radiation. These microcrystals stayed reliable, with their properties changing by only 0.5% or 0.05%, even after being hit with a high level of neutron radiation (1 x 10^15 neutrons per square centimetre). This experiment confirmed a theory that the properties of irradiated materials don't depend on their history, like how they were made or what impurities were added.

1.3. About GEANT4

Introduction to Geant4

Geant4, short for Geometry and Tracking, is a software toolkit developed for simulating the passage of particles through matter. It is primarily used in the fields of high energy physics, nuclear experiments, medical applications, and space science. The toolkit is designed to be versatile, allowing users to simulate complex interactions involving various types of particles and materials.

Origins and Development

Geant4 was developed by a collaboration of physicists and engineers from around the world. It was first released in 1998, building on the experience and knowledge gained from its predecessor, Geant3. The development of Geant4 was motivated by the need for a more flexible and extensible simulation platform that could adapt to the rapidly evolving requirements of modern scientific research.

Purpose and Scope

The primary purpose of Geant4 is to provide a simulation environment that is as close to reality as possible. This capability is crucial for scientists and engineers who rely on accurate predictions of particle behavior under different conditions. Whether it's designing a new particle detector, planning a medical treatment with radiation, or simulating cosmic rays in space, Geant4 offers the tools necessary to model these complex phenomena accurately.

Key Features

The toolkit is renowned for its comprehensive set of features that enable detailed simulation of complex scenarios:

- **Particle Tracking**: Geant4 can simulate the trajectory of particles as they pass through different materials, accounting for various physical processes such as scattering and absorption.
- **Physics Processes**: It includes a wide range of models to describe the interactions of particles with matter, including electromagnetic, hadronic, and optical processes.
- **Event and Run Management**: Geant4 allows for the simulation of numerous events in a controlled manner, facilitating the study of statistical variations and rare occurrences.

Impact on Research and Industry

Since its inception, Geant4 has had a profound impact on both academic research and industrial applications. It has become a standard tool in particle physics experiments and is extensively used in medical physics for imaging and radiation therapy planning. Additionally, its applications in aerospace engineering have helped in designing better shielding materials against cosmic radiation, enhancing the safety and reliability of space missions.

This introduction sets the stage for a deeper exploration of Geant4's capabilities, architecture, and applications in subsequent sections of the chapter. It highlights the toolkit's significance and versatility, underscoring its role as an indispensable resource in various scientific and engineering disciplines.

Core Features and Software Architecture of Geant4

Geant4 is distinguished by its comprehensive suite of features that enable detailed and accurate simulations of particle interactions with matter. This section delves into the core capabilities that make Geant4 a powerful tool in scientific research and industrial applications.

Physics Models

Geant4 includes a wide array of physics models that cover a broad spectrum of interactions and phenomena:

- **Electromagnetic Interactions**: The toolkit provides detailed models for electromagnetic processes including ionization, bremsstrahlung, pair production, and photon scattering. These models are crucial for simulations involving electrons, positrons, and photons.
- **Hadronic Interactions**: Geant4 offers models for interactions involving hadrons, such as protons, neutrons, and pions. These include elastic scattering, inelastic scattering, and nuclear reactions, which are essential for nuclear physics experiments and applications.
- **Optical Processes**: The toolkit also simulates optical processes like Cherenkov radiation, scintillation, and the absorption and re-emission of photons, which are important in the design of optical detectors.

Geometry and Material Handling

Geant4 allows users to define complex geometries and a variety of materials:

- **Geometric Modeling**: Users can construct detailed geometric models of experimental setups, including various shapes and volumes. This feature is vital for accurately simulating the physical environment in which particle interactions occur.
- **Material Definition**: The toolkit supports a comprehensive library of materials and allows for custom material definitions. Each material can be characterized by properties such as density, atomic number, and radiation length, which are critical for simulating particle interactions.

Tracking and Event Management

Geant4 excels in tracking particles through materials and managing simulation events:

- **Particle Tracking**: The toolkit tracks the trajectory of each particle through different materials, calculating the interactions and transformations that occur along the way. This includes the generation of secondary particles and the handling of their subsequent interactions.
- **Event Simulation**: Geant4 can simulate a large number of events, which is essential for statistical analyses in experiments. It allows for the configuration of initial conditions and control over the simulation parameters, enabling detailed studies of specific scenarios.

Visualization and User Interface

Geant4 provides several options for visualizing simulations.

- **Visualization Tools**: The toolkit includes various visualization drivers that allow users to see the geometry of the experimental setup and the paths of particles in real-time. This is useful for debugging and for educational purposes.

- **User Interface**: Geant4 offers both graphical and command-line interfaces. The graphical user interface (GUI) is user-friendly and suitable for setting up and monitoring simulations interactively, while the command-line interface is ideal for batch processing and automation.

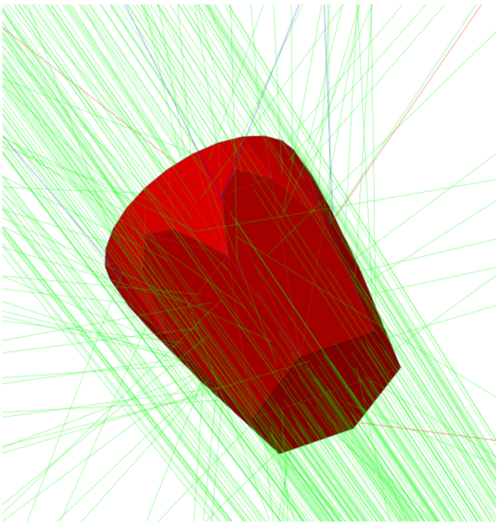


Figure. 1.7. - Example of visualization in Geant software

Community and Documentation

Geant4 is supported by a robust community and extensive documentation:

- **Active Community**: The Geant4 user community is active and global, consisting of developers and users from various fields. This community contributes to the continuous improvement of the toolkit and provides support through forums and workshops.

- **Comprehensive Documentation**: Geant4 comes with detailed documentation, including manuals, tutorials, and example applications, which are invaluable resources for new and experienced users alike.

These core features and capabilities make Geant4 a versatile and indispensable tool in fields ranging from high-energy physics to medical imaging and space science. The toolkit's ability to simulate complex particle interactions with high accuracy is crucial for advancing research and development in these areas.

Software Architecture of Geant4

The software architecture of Geant4 is designed to be highly modular and flexible, enabling it to accommodate a wide range of simulation needs across different scientific disciplines. This architecture not only supports complex and varied simulation tasks but also allows for customization and extension by users. Here, we explore the key components and design principles that define the Geant4 software architecture.

Extensibility

A key feature of Geant4's architecture is its extensibility:

- **Plugin Mechanism**: Users can develop their own modules or plugins to extend the functionality of Geant4. This can include new physics processes, custom materials, or specialized tracking algorithms.
- **APIs and Interfaces**: Geant4 exposes a set of APIs and interfaces that allow users to interact with and extend the toolkit. These interfaces are well-documented, facilitating the integration of Geant4 into larger software frameworks or its adaptation to specific research needs.

Modular Design

Geant4's architecture is fundamentally modular, composed of several independent but interrelated modules that handle different aspects of the simulation process:

- **Physics Modules**: These are responsible for defining the physical processes that can occur during particle interactions, such as electromagnetic, hadronic, and optical processes. Each physics process is encapsulated in its own module, allowing users to select and combine different physics models as needed for their specific simulation requirements.
- **Geometry Module**: This module manages the spatial configuration of the simulation, including the definition of the shapes, volumes, and materials of the objects involved. It allows for the construction of complex geometrical setups from simple predefined shapes to complex user-defined structures.
- **Tracking Module**: Central to Geant4, this module handles the propagation of particles through the simulation geometry. It tracks the trajectory of each particle, calculates interactions with materials, and manages the generation and tracking of secondary particles.
- **Event Management Module**: This module controls the simulation of events, where an event is defined as a single instantiation of the initial conditions of a simulation run. It manages the sequence of events and ensures that the statistical sampling is representative of the physical scenario being modeled.

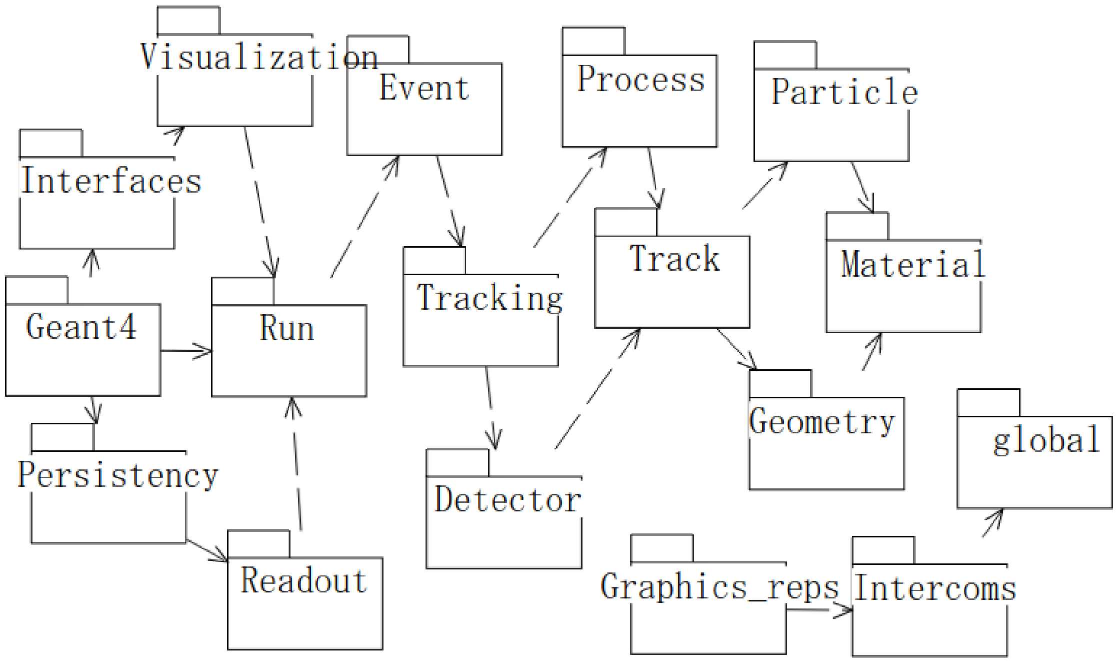


Figure. 1.8 - Flow diagram of GEANT-4 Functionality

Kernel and Manager Classes

At the core of Geant4's architecture is the kernel, which integrates various components of the toolkit:

- **Run Manager**: The Run Manager is the central controller that initializes the simulation, processes all events, and terminates the simulation. It orchestrates the interaction between different modules and ensures that the simulation proceeds correctly.

- **Event Manager**: This component is responsible for generating and managing individual events within a simulation run. It interacts closely with the tracking module to process all particles within an event.

- **Geometry Manager**: This manager is tasked with handling all aspects of the simulation geometry, ensuring that the physical layout and material properties are correctly implemented and maintained throughout the simulation.

The architecture of Geant4 is a reflection of its design philosophy to provide a robust, flexible, and user-friendly toolkit for simulating the interaction of particles with matter across a wide range of applications. Its modular design, combined with extensive documentation and community support, ensures that Geant4 remains adaptable to the evolving needs of the scientific community.

Key Strengths of Geant4

- **Versatility**: One of Geant4's most significant advantages is its versatility. It can simulate a vast array of physical processes and interactions, making it applicable to many different fields and research questions.
- **Modularity and Customizability**: The modular architecture of Geant4 not only allows users to select and configure the components that are most relevant for their specific needs but also makes it possible to extend the toolkit by adding new models and functionalities.
- **Active Community and Support**: Geant4 benefits from a robust and active community. This community not only contributes to the continuous development and improvement of the toolkit but also provides substantial support through forums, workshops, and documentation, aiding both new and experienced users.

Challenges and Limitations

- **Complexity and Learning Curve**: The flexibility and power of Geant4 come with a complexity that can be daunting for new users. The steep learning curve may require significant investment in time and resources to overcome.
- **Performance Considerations**: For certain applications, especially those involving very complex geometries or large numbers of particles, Geant4 simulations can be computationally intensive and time-consuming.

Future Directions

Looking forward, the development of Geant4 is likely to continue addressing both the expansion of its capabilities and the usability of the software. Efforts may focus on:

- **Enhancing User-Friendliness**: Simplifying the interface and streamlining the configuration process could make Geant4 more accessible to a broader audience and reduce the entry barrier for new users.
- **Optimizing Performance**: As computational demands grow, especially in large-scale simulations, there will be an ongoing need to optimize Geant4's performance to handle larger datasets and more complex simulations efficiently.
- **Expanding Applications**: As new scientific and technological challenges arise, Geant4 will likely continue to expand its range of applications, possibly venturing into emerging fields such as nanotechnology, quantum computing, or even more specialized areas of biomedical research.

Conclusion

In conclusion, Geant4 is a critical tool that has significantly contributed to advancements in multiple scientific fields. Its development reflects the collaborative efforts of a global community of researchers and developers. As technology and science continue to advance, Geant4 will undoubtedly evolve, further cementing its role as a cornerstone tool in scientific research and industrial applications. The ongoing development and adaptation of

Geant4 will ensure that it remains at the forefront of simulation technology, ready to meet the challenges of tomorrow's scientific inquiries and technological innovations.

2. EXPERIMENT

2.1. Why is the experiment important

Geant4 is a robust toolkit utilized for simulating the trajectories of particles through substances, particularly excelling in the simulation of neutron interactions. The toolkit's extensive use can be attributed to various fundamental factors. One primary rationale is the substantial cost and intricate nature of experimental configurations. The execution of physical experiments to investigate neutron interactions can prove excessively expensive, often necessitating specialized infrastructures such as nuclear reactors or particle accelerators. These facilities not only demand significant financial investments for construction and maintenance but also for operational expenses. Furthermore, the implementation of safety procedures for managing radioactive substances introduces an additional layer of complexity and cost.

Moreover, physical experiments are time-intensive, encompassing not only the duration of the experiment itself but also the preparatory and analytical phases. Establishing an experiment to analyze neutron interactions requires meticulous planning to ensure precise outcomes, with subsequent data interpretation being equally laborious. Geant4, conversely, circumvents these logistical challenges by offering a virtual platform where diverse scenarios can be replicated and examined with relative ease. This approach not only saves time but also facilitates an extensive exploration of parameters and conditions that may be impractical or unfeasible to replicate physically.

Additionally, Geant4 boasts exceptional precision and adaptability. It integrates intricate models of neutron interactions across various energy spectrums, enabling simulations that closely mirror real-world scenarios. Researchers can customize these models to suit their specific requirements, modifying variables and circumstances to align with their investigative goals. This level of detail and flexibility positions Geant4 as an indispensable tool in fields like medical physics, where it enhances the optimization of cancer treatments involving neutron beams, and in aerospace engineering, enabling the assessment of cosmic radiation effects on spacecraft materials and electronics.

Ultimately, Geant4 presents a versatile and cost-efficient alternative to physical experiments, empowering scientists and engineers to conduct thorough investigations of neutron interactions with matter without the accompanying financial burdens and logistical complexities. Its capability to simulate intricate scenarios with precision renders it an invaluable asset in advancing our comprehension of neutron behavior and its diverse applications across scientific domains.

2.2. Parameters of simulation

Importance of the Study

While considerable research has been conducted on the radiation resistance of electronic devices, less attention has been given to the semiconductor materials themselves. Understanding the effects of ionizing radiation on these materials is essential, as changes in device parameters due to radiation are often insufficient to reveal the underlying mechanisms of radiation damage.

Simulation Environment

Given the extensive duration required for physical experiments, the Geant4 simulation software was employed to model the interactions within the semiconductor. Geant4 utilizes the Monte Carlo method to simulate the random interactions of particles with matter, supporting a variety of particles including electrons, protons, alpha particles, neutrons, and gamma rays.

Material Specifications

The simulations were conducted on a target modeled as a parallelepiped with a volume of 1 cm^3, composed of bulk pure InAs material. The specific parameters of the InAs material used in the simulations were as follows:

Density: 5.670 g/cm^3;
Radiation Length: 1.741 cm;
Nuclear Interaction Length: 28.273 cm;
Mean Ionization Energy (Imean): 424.674 eV;
Temperature: 293.15 K;
Pressure: 1.00 atm;

Table#1. Isotopes and abundances of elements in the target material

Element	N	ElmMassFraction, %	Abundance, %	ElmAbundance, %
In	113	60	5	49.46
	115		95	
As	75	40	100	50.54

Physics Models and Parameters

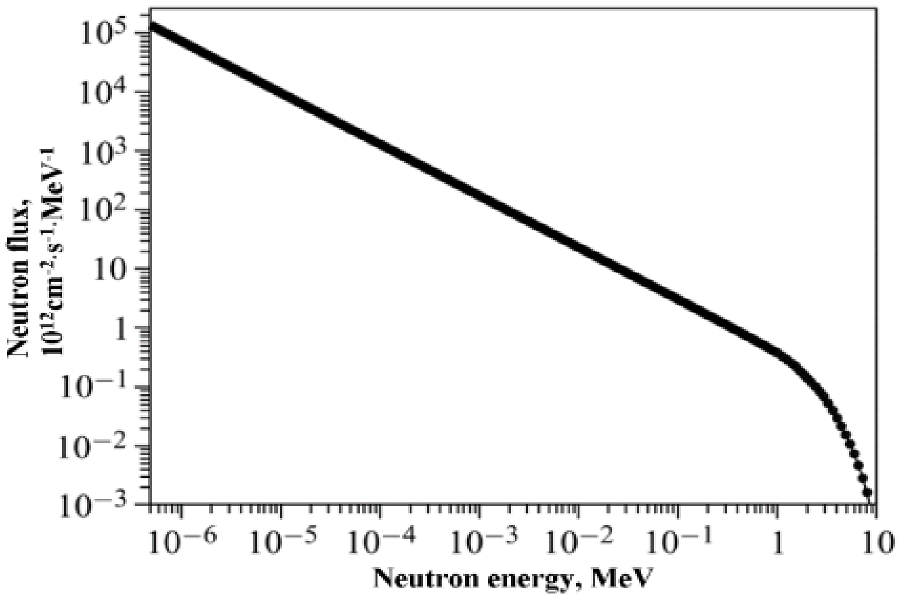
The Geant4 toolkit was utilized to simulate the interaction of neutrons with the InAs semiconductor material. The physics model chosen for this purpose was the QGSP_BIC_HP (Quark-Gluon String Precompound Binary Cascade High Precision) model, which is part of Geant4's standard package of physics lists. This model is particularly suited for simulating interactions involving neutrons and provides a comprehensive description of the following processes:

- **Elastic Scattering:** This process involves the scattering of neutrons by nuclei without any energy transfer that would excite the nucleus. It is crucial for understanding how neutrons propagate through a material and their potential to reach sensitive regions within electronic devices.

- **Inelastic Scattering:** In this process, neutrons transfer part of their energy to the nucleus, exciting it to a higher energy state. The excited nucleus can emit gamma rays or other particles as it returns to its ground state, which can significantly affect the material's electronic properties.
- **Pre-equilibrium States:** Before reaching equilibrium, the system may pass through various pre-equilibrium states where the distribution of energy among particles is non-thermal. This model accounts for such states, which are important in high-energy interactions.
- **String and Hadronic Radiation:** These processes involve the formation of quark-gluon strings and their subsequent decay into hadrons, which are critical for understanding high-energy neutron interactions within the nucleus.
- **Secondary Particle Cascades:** The interactions can produce secondary particles, which themselves initiate further interactions, leading to a cascade effect. This is vital for assessing the cumulative impact of neutron irradiation on semiconductor materials.

The cross-sectional data for neutron interactions were sourced from the JENDL-4.0 (Japanese Evaluated Nuclear Data Library) open-source data library, ensuring high accuracy and reliability of the simulation results.

Each target was virtually irradiated with neutrons arriving perpendicular to the surface with energy equal to 0.0253 eV, 14 MeV, and the Maxwell spectrum of reactor experimental neutron energy spectrum of the IBR-2 channel No.3 at a distance of 30 mm from the water moderator (Figure 1).



Picture 2.1- Differential energy density of neutron flux in channel No. 3 of the IBR-2 reactor at a distance of 0.3 m from the water moderator.

Reactions of Material Nuclei with Neutrons

An in-depth analysis was conducted to understand the various nuclear reactions that can occur within the indium arsenide (InAs) material when its nuclei interact with neutrons. This analysis focused on the cross sections of these reactions at different neutron energies, the intermediate and final isotopes formed, and their respective half-lives.

Each of these elements can undergo several types of nuclear reactions upon neutron irradiation. The primary reactions considered in this study include neutron capture (n,γ), neutron inelastic scattering (n,n'γ), and transmutation reactions leading to different isotopes.

The transmutation of nuclei due to neutron capture can lead to the formation of new elements within the semiconductor matrix. For instance, the beta decay of Indium-114 to Tin-114 and Arsenic-76 to Selenium-76 introduces new chemical elements into the InAs lattice. These transmutations can alter the electronic properties of the material, potentially leading to degradation or failure in semiconductor devices.

Table#2. Basic reactions of interaction of the studied elements with a neutron [JENDLE site].

Materials	**Reaction**	**Cross section К = 0,025 eV**	**Resonance cross section**	**Fast cross section**	**Element**	**exemplary T1/2**	**Total element**
As75	n,g	4,15	63,74	9,82E-04	As76	1d	Se76
	n,a	-	7,82E-04	9,82E-03			
	n,inelastic	-	-	6,45E-01			
	n,2n	-	-	9,39E-01	As74	17d	Se74, Ge74
	n,inelastic	-	3,93	3,96E-01			
	n,2n	-	-	1,16E+00	Ge75	1h	As75
In113	n,g	12,09	3,25E+02	1,14E-06	In114	1,2m	Sn114
	n,p	-	1,57E-03	3,96E-02			
	n,inelastic	-	-	4,88E-01			
	n,2n	-	-	1,48E+00	In112	14,97m	Cd112, Sn112
	n,a	-	7,75E-05	3,38E-03			
In115	n,g	201,20	3209,00	9,48E-04	In116	54min	Sn116
	n,inelastic	-	-	4,32E-01			
	n,2n	-	-	1,56E+00	In114	1,2m	Sn114
	n,a	-	2,26E-05	1,88E-03			

The transmutation of nuclei due to neutron capture can lead to the formation of new elements within the semiconductor matrix. For instance, the beta decay of Indium-114 to Tin-114 and Arsenic-76 to Selenium-76 introduces new chemical elements into the InAs lattice. These transmutations can alter the electronic properties of the material, potentially leading to degradation or failure in semiconductor devices.

Tin (Sn) and Selenium (Se) incorporation into the lattice can introduce defects, change carrier concentrations, and affect the band structure, impacting the semiconductor's optical and electrical properties.

This analysis helps in predicting the behavior of InAs-based devices in radiation-rich environments and guides the development of more robust materials for such applications. The cross-sectional data and reaction products analyzed in this chapter are essential for modeling the long-term effects of neutron irradiation on semiconductor heterostructures.

3 RESULTS

3.1. Reactions within the material under the influence of high energy neutron irradiation

When high-energy neutrons interact with semiconductor materials, they transfer part of their kinetic energy to the atoms of the material. This energy transfer can displace atoms from their original positions in the crystal lattice, leading to the formation of defects in the crystal structure. This phenomenon is illustrated in figures [3.1. – 3.2.]. Figure [3.1] shows the dependence of the number of interactions on the kinetic energy of the In113 particle. Contrary to the initial description, we would expect an increase in certain interaction types, such as inelastic scattering, with increasing kinetic energy, up to a certain threshold. Figure [3.2] for the In115 particle should similarly reflect this trend, depending on the specific interaction cross-sections involved.

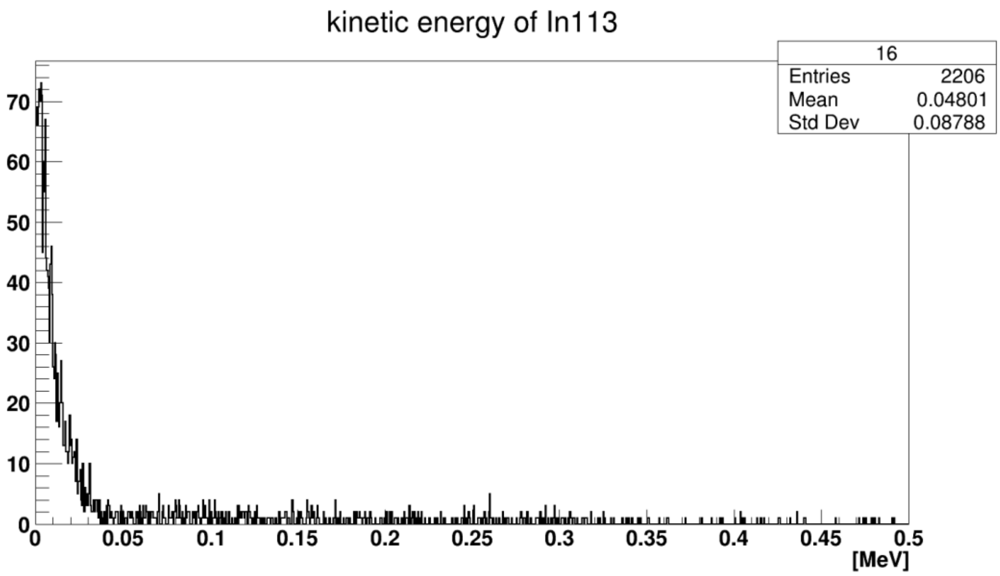


Figure. 3.1. - The losses in kinetic energy in In113 particles when irradiated with a neutron flux of 14 MeV energy.

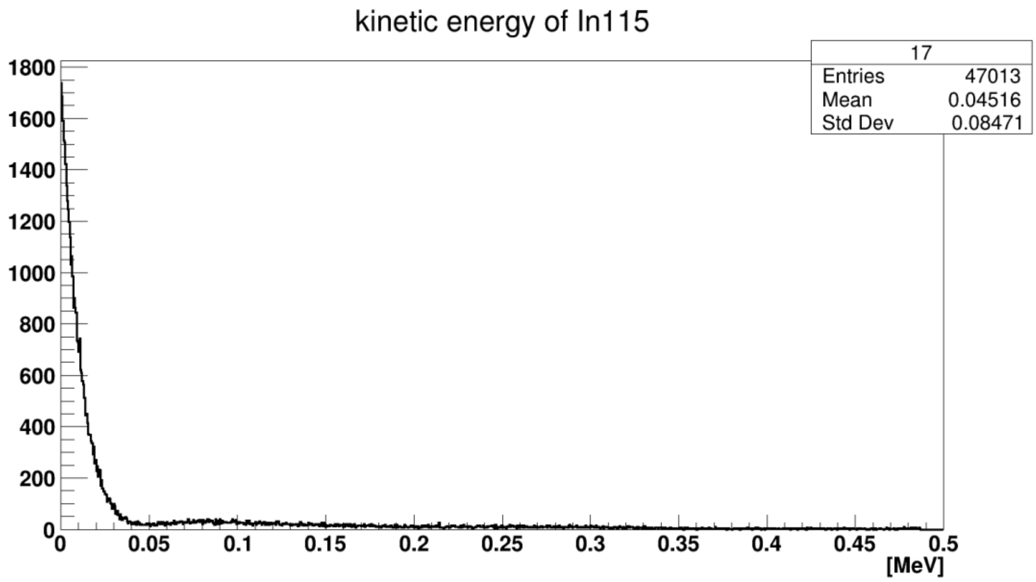


Figure. 3.2. - The losses in kinetic energy in In115 particles when irradiated with a neutron flux of 14 MeV energy.

Figure [3.3] shows the distribution of different types of reactions. It is observed that the number of inelastic and elastic scattering events significantly exceeds the number of neutron captures at the neutron energy of 14 MeV. This is due to the higher cross-sections for elastic and inelastic scattering at this energy, compared to neutron capture, which typically has lower cross-sections at higher energies.

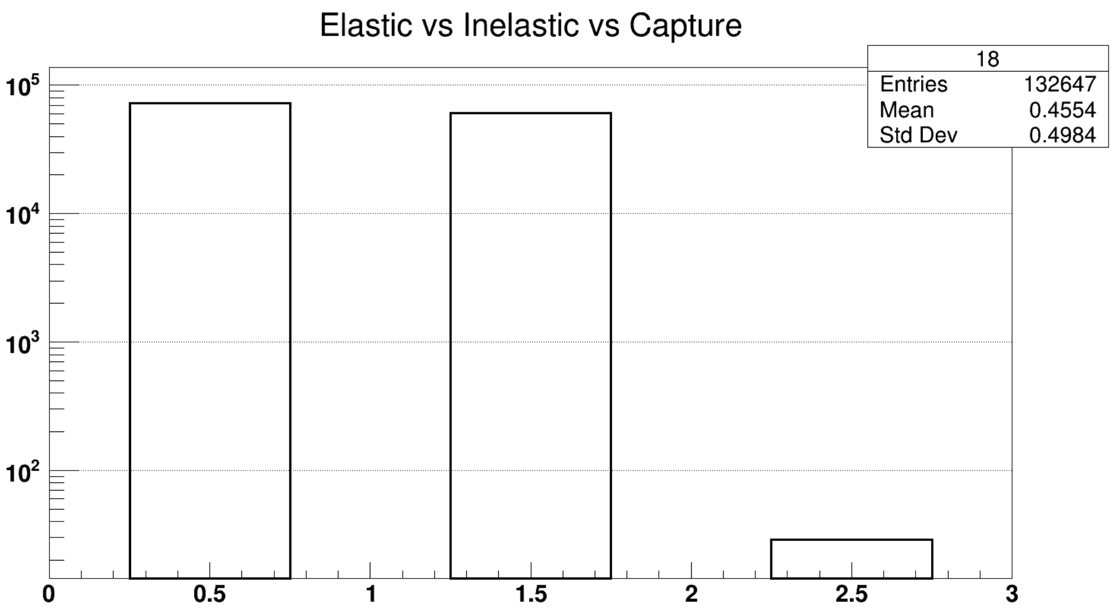


Figure. 3.3. - The percentage distribution of reactions at a neutron energy of 14 MeV.

Figure [3.4] illustrates the distribution of secondary particles formed as a result of exposure to high-energy neutron radiation. Indium (In) and arsenic (As) are elements in the semiconductor material, and the defects typically include vacancies or interstitials caused by the displacement of these atoms. Other secondary particles such as alpha particles, protons, and deuterons, while also acting as charge carriers, play significant roles in lattice damage and ionization, impacting the semiconductor's electronic properties.

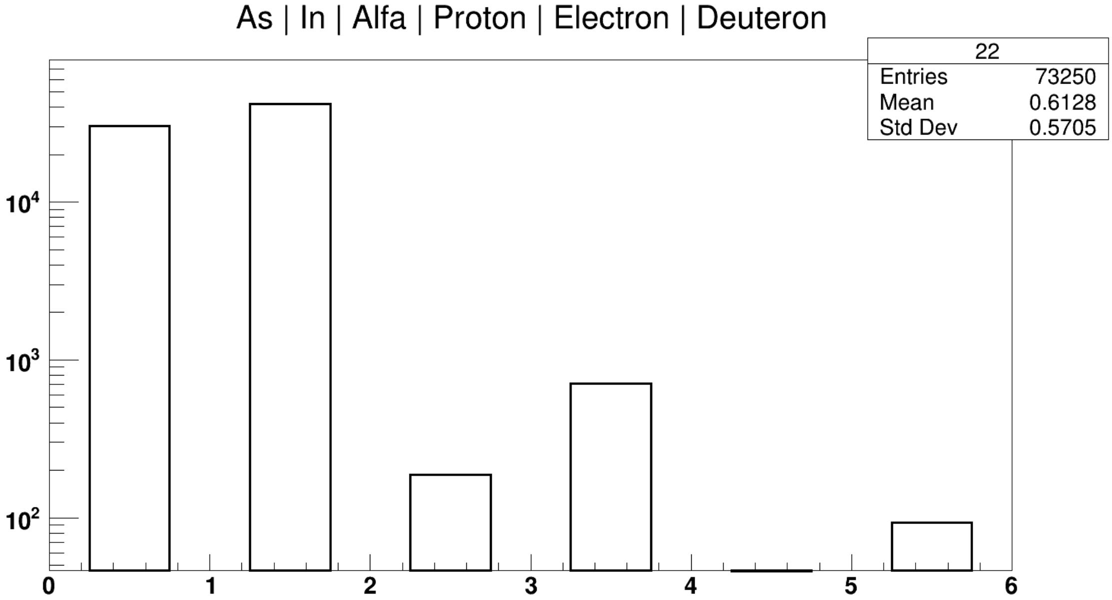


Figure. 3.4. - The percentage distribution of reactions at a neutron energy of 14 MeV.

Figure [3.5] demonstrates that the energy distribution as a result of elastic scattering varies with the scattering angle and the masses of the particles involved. The absence of significant peaks in the graph indicates a broad range of scattering angles or a uniform angular distribution, rather than a uniform distribution of energy.

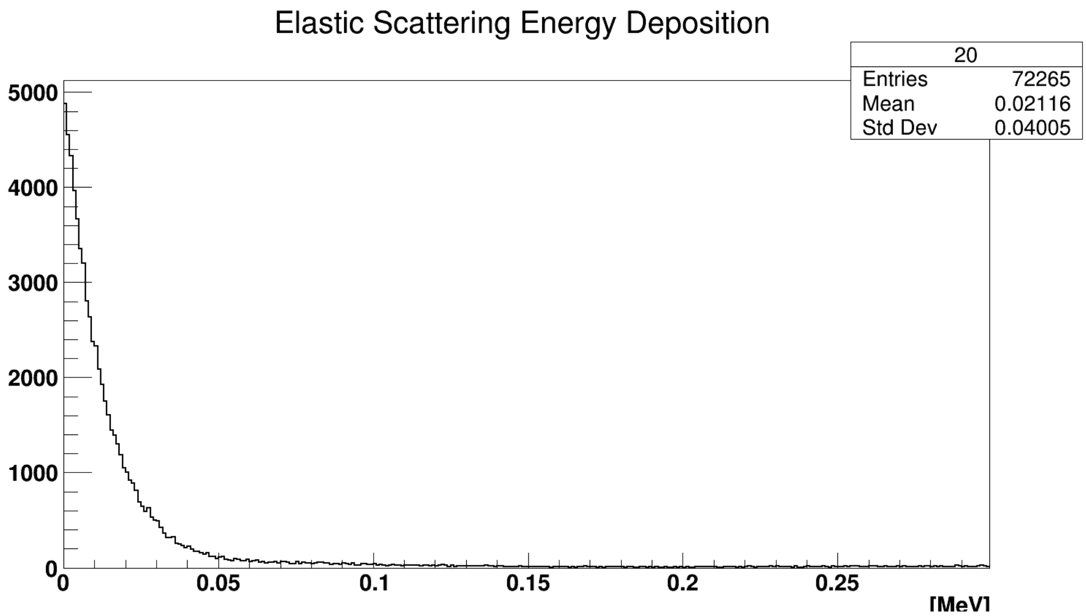


Figure. 3.5. - Elastic Scattering Energy Deposition

Figure [3.6] shows that inelastic scattering leads to a noticeable energy transfer, which is confirmed by the presence of a pronounced peak in the graph. This peak indicates the specific energy at which the material accumulates energy, causing the excitation or emission of particles, characteristic of inelastic interactions.

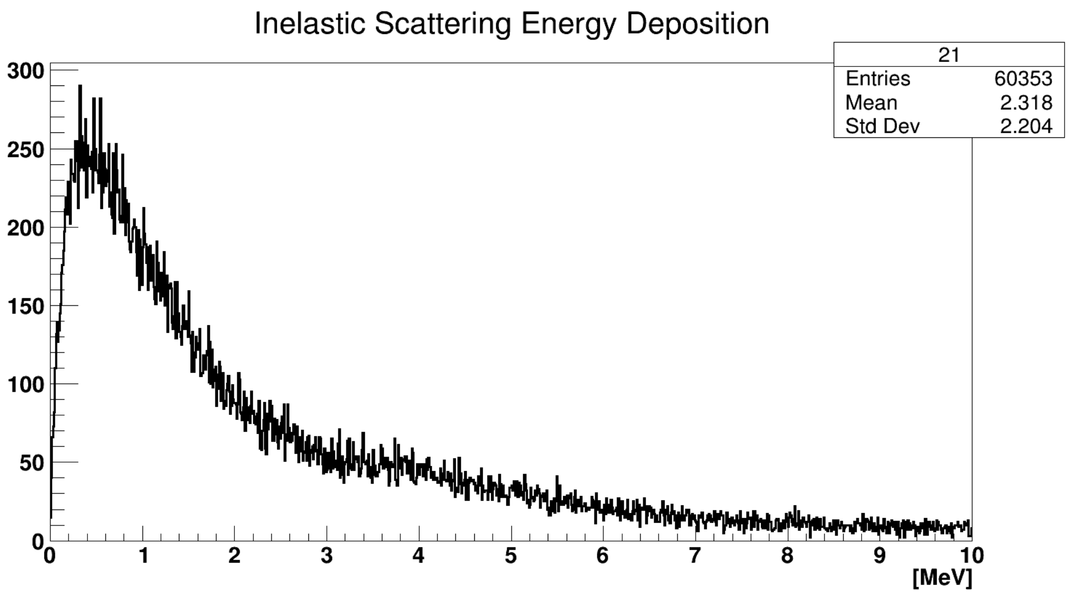


Figure. 3.6. Inelastic scattering energy deposition

3.2. Reactions within the material under the influence of thermal neutron irradiation

When thermal neutrons interact with semiconductor materials, they primarily engage in neutron capture rather than transferring kinetic energy to the atoms of the material, as thermal neutrons have very low kinetic energy. This process can lead to the formation of defects in the crystal structure due to the transmutation of atoms and the subsequent displacement of neighboring atoms in the crystal lattice. This phenomenon is illustrated in figures [3.7 – 3.9]. Figure [3.7] should show the dependence of the number of neutron capture events on the kinetic energy of the In113 isotope. Since thermal neutrons have energies around 0.0253 eV, the interaction cross-section for neutron capture is significantly higher, which is why we observe an increase in capture events at these energies. Figures [3.8 – 3.9] should reflect similar trends for other isotopes or materials, depending on their specific neutron capture cross-sections.

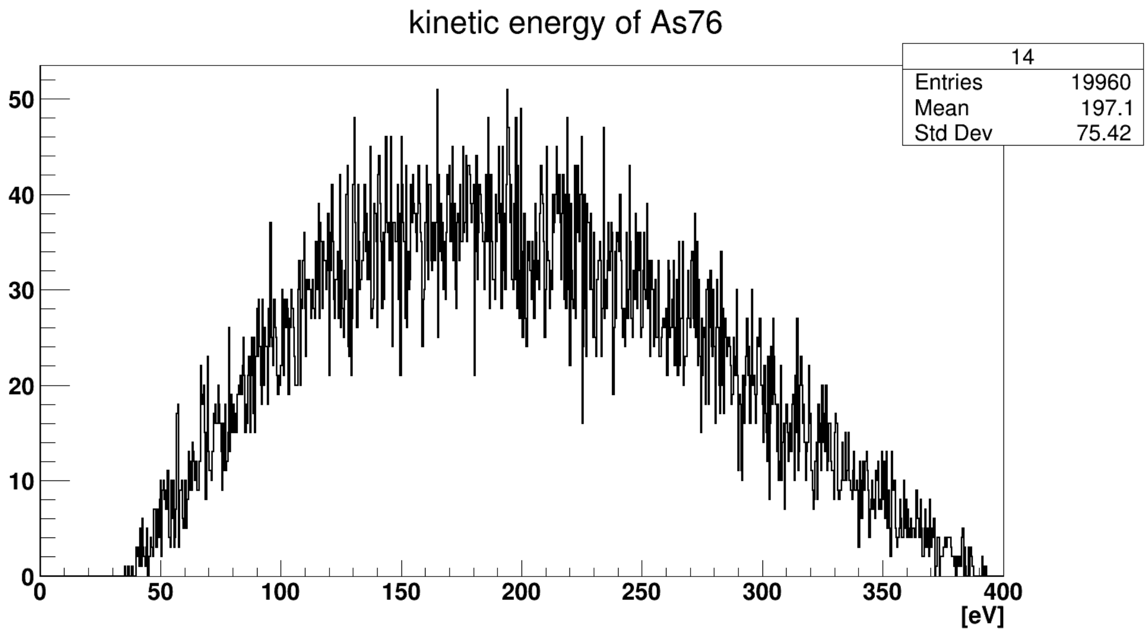


Figure. 3.7. The losses in kinetic energy in As76 particles when irradiated with a neutron flux of 0.0253 eV energy.

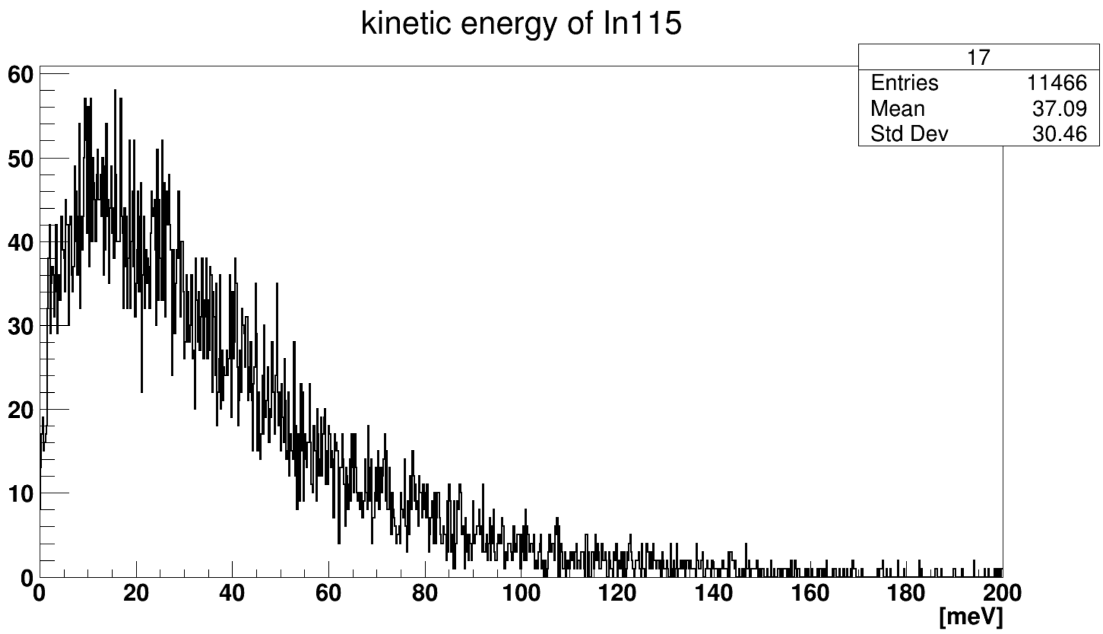


Figure. 3.8. The losses in kinetic energy in In115 particles when irradiated with a neutron flux of 0.0253 eV energy.

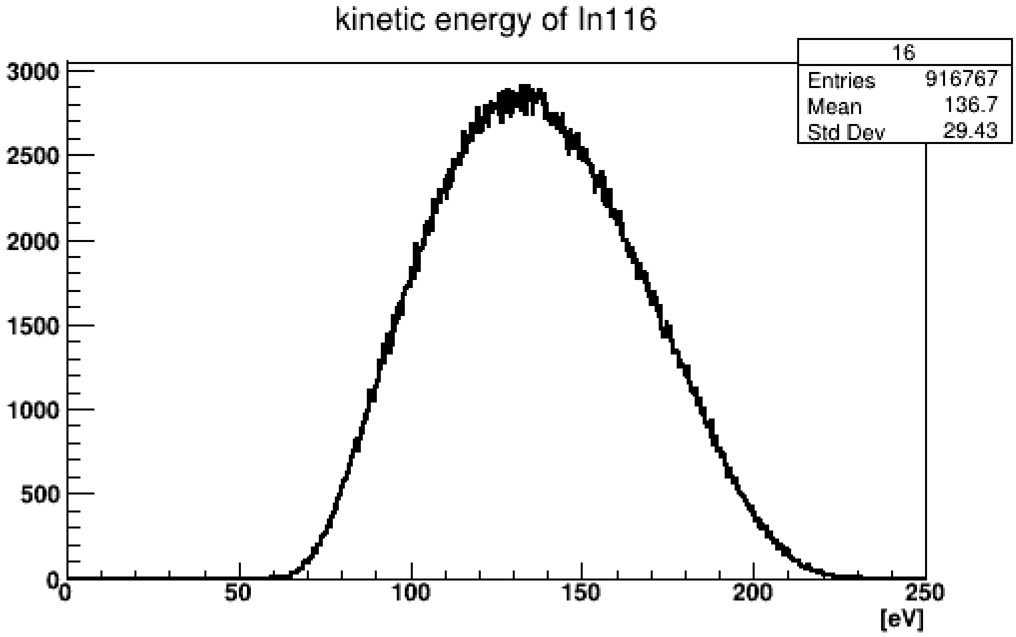


Figure. 3.9. The losses in kinetic energy in In116 particles when irradiated with a neutron flux of 0.0253 eV energy.

Figure [3.10] shows that at the energy of thermal neutrons (0.0253 eV), the number of inelastic and elastic scattering events is significantly lower than the number of neutron captures. This is due to the much higher cross-sections for neutron capture at thermal energies compared to those for elastic and inelastic scattering.

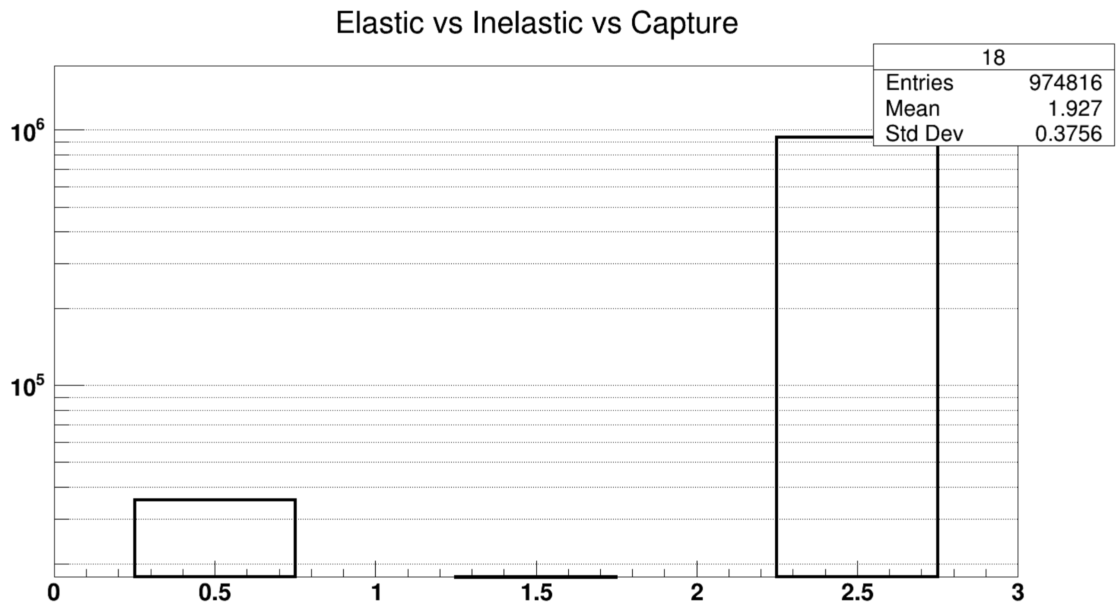


Figure. 3.10. The percentage distribution of reactions at a neutron energy of 0.0253 eV.

Figure [3.11] illustrates the distribution of secondary particles formed as a result of neutron capture. The formation of secondary particles such as alpha particles, protons, and deuterons typically results from reactions following neutron capture, such as (n,α) or (n,p) reactions, and these particles can indeed cause significant lattice damage and ionization.

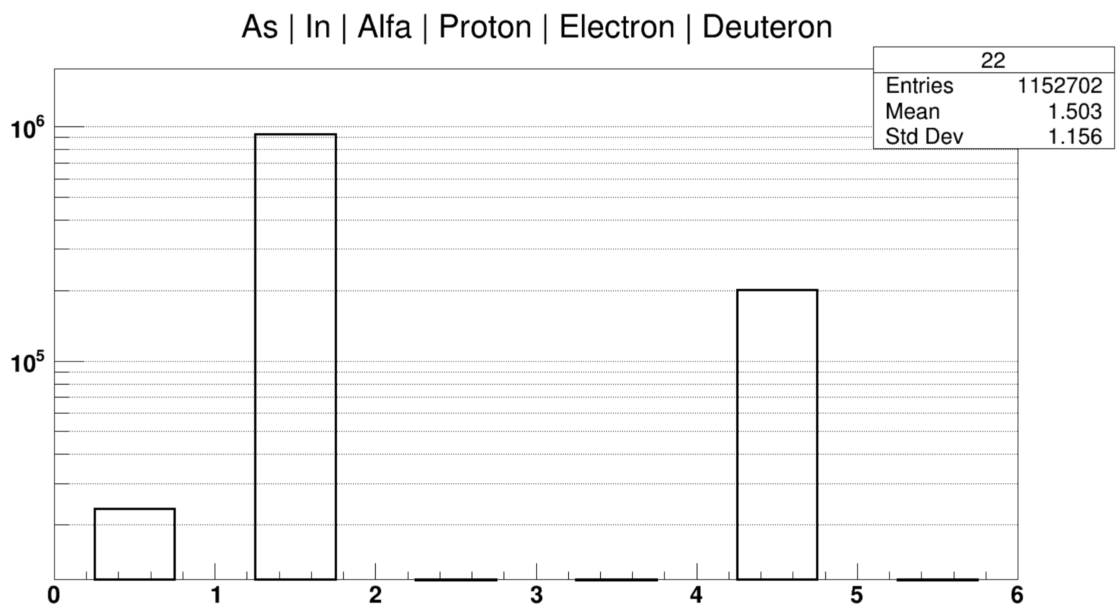


Figure. 3.11. The percentage distribution of reactions at a neutron energy of 0.0253 eV.

Figure [3.12] demonstrates the energy distribution resulting from the neutron capture process. Neutron capture typically leads to the emission of gamma rays and the creation of a new isotope, which may itself be unstable. Due to the low occurrence of elastic and inelastic scattering at thermal neutron energies, the energy distributions for these processes are minimal and are not included in the report.

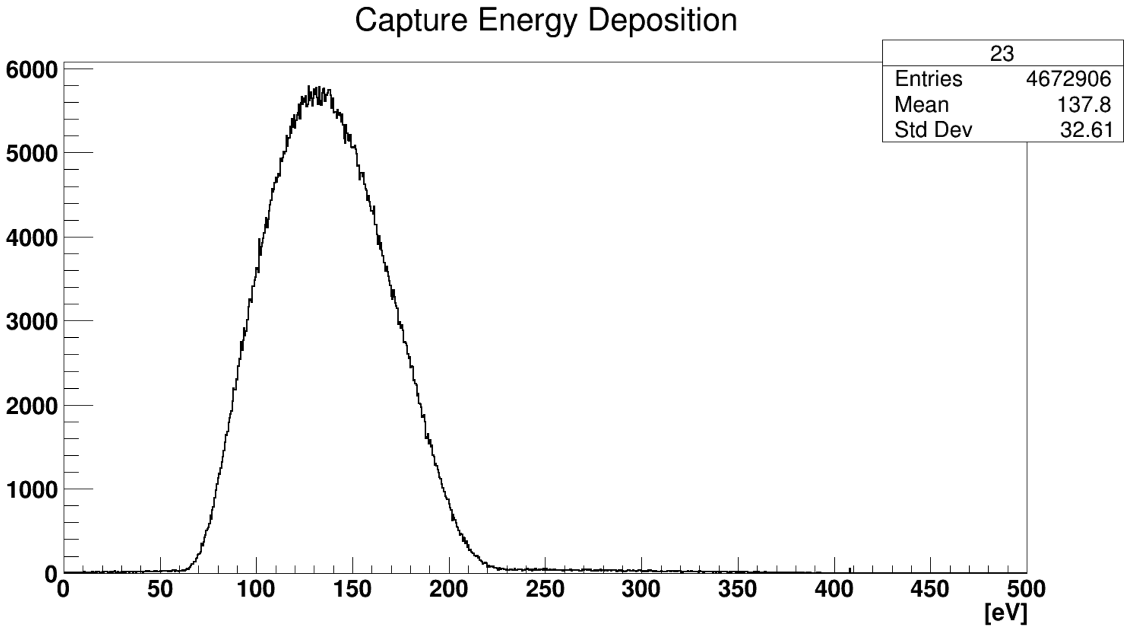


Figure. 3.12. Neutron capture energy deposition

3.3 Reactions within the material under the influence of spectrum of neutron irradiation

When a spectrum of neutrons interacts with semiconductor materials, it transfers part of its kinetic energy to the atoms of the material. This energy transfer can displace atoms from their original positions in the crystal lattice, leading to the formation of defects in the crystal structure. This phenomenon is illustrated in Figures [3.13 – 3.16]. Figure [3.13] shows the dependence of the number of interactions on the kinetic energy of the As-76 particle. Contrary to the initial description, we would expect an increase in certain types of interactions, such as neutron capture, elastic scattering, and inelastic scattering, with increasing kinetic energy, up to a certain threshold. Neutron capture, as well as both elastic and inelastic scattering, will be present because we are dealing with a neutron spectrum that has a distribution of different energies. Figures [3.14 – 3.16] should similarly reflect this trend, depending on the specific interaction cross-sections involved.

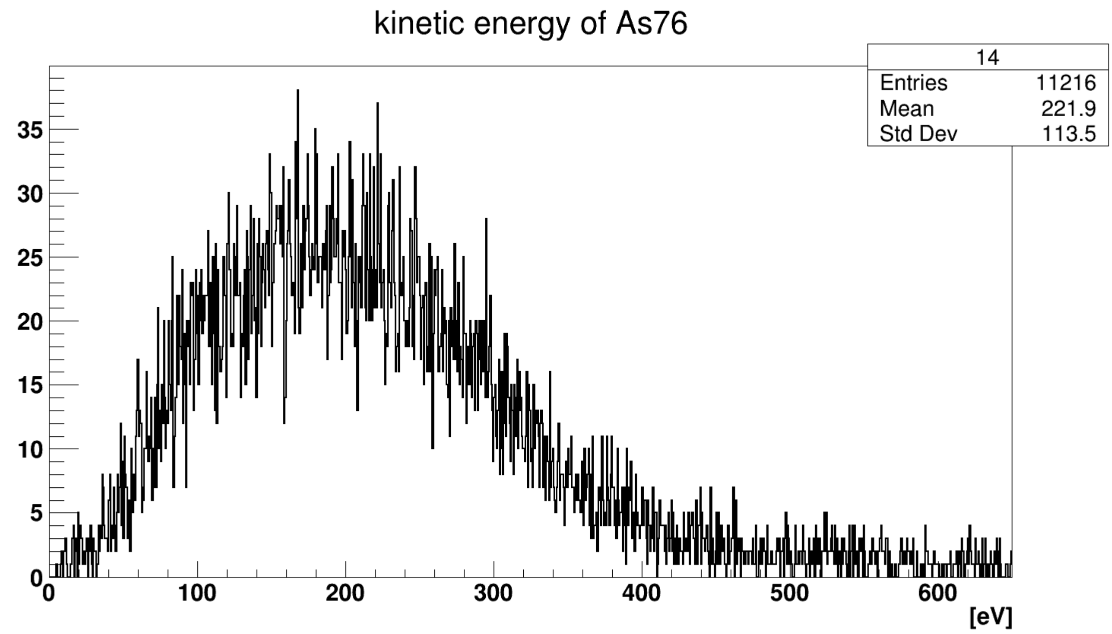


Figure. 3.13. The losses in kinetic energy of As-76 particles when irradiated with a neutron flux spanning a spectrum of energies.

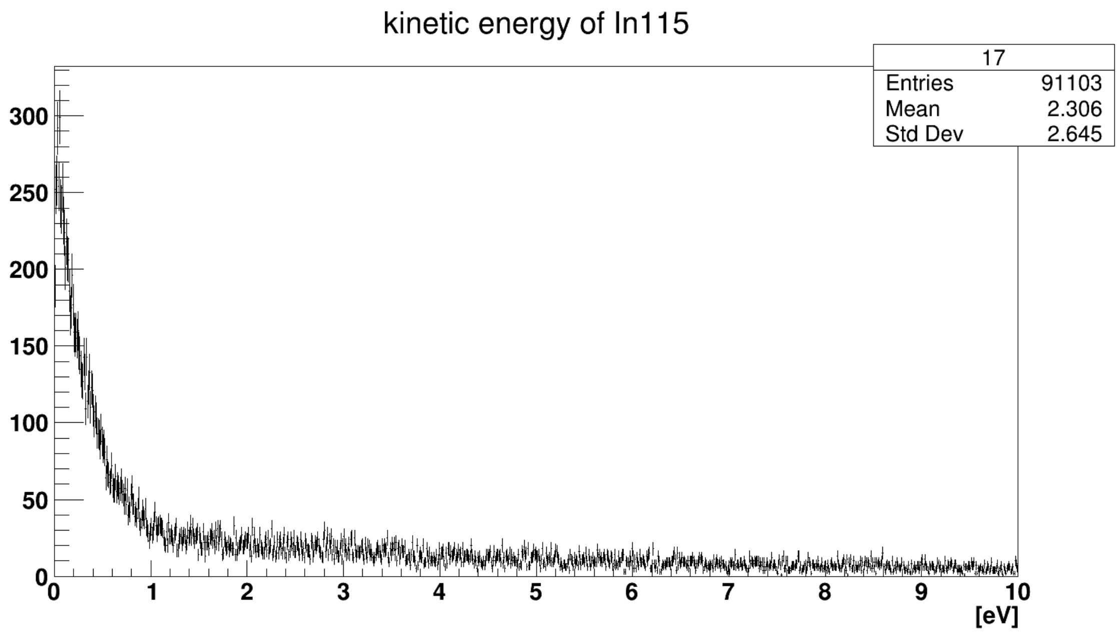


Figure. 3.14. The losses in kinetic energy of In-115 particles when irradiated with a neutron flux spanning a spectrum of energies.

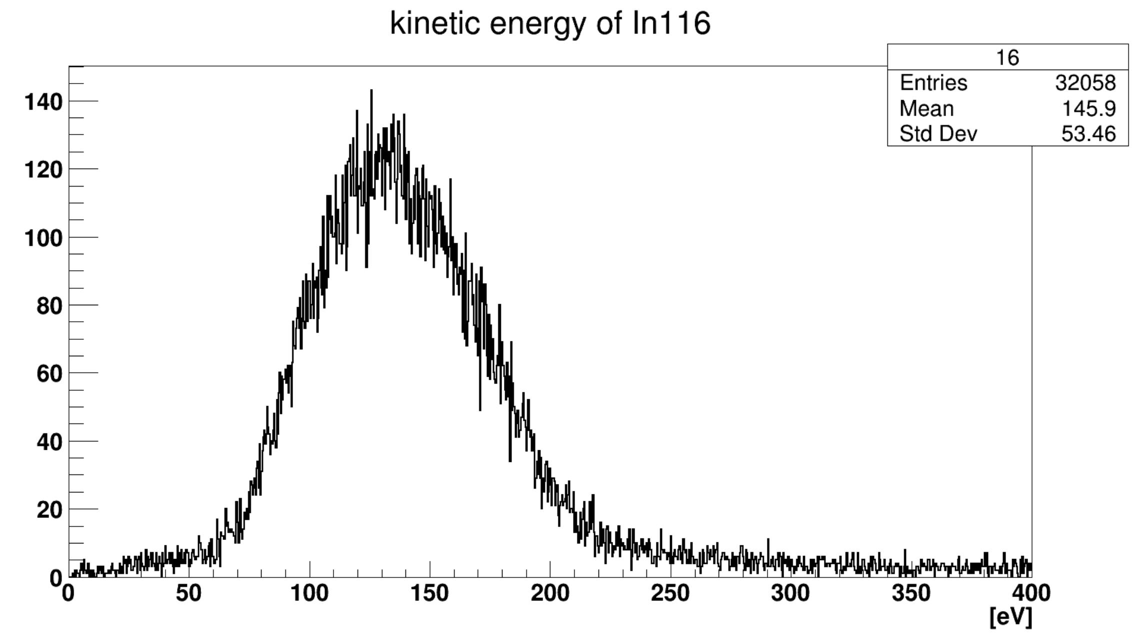


Figure. 3.15. The losses in kinetic energy of In-116 particles when irradiated with a neutron flux spanning a spectrum of energies.

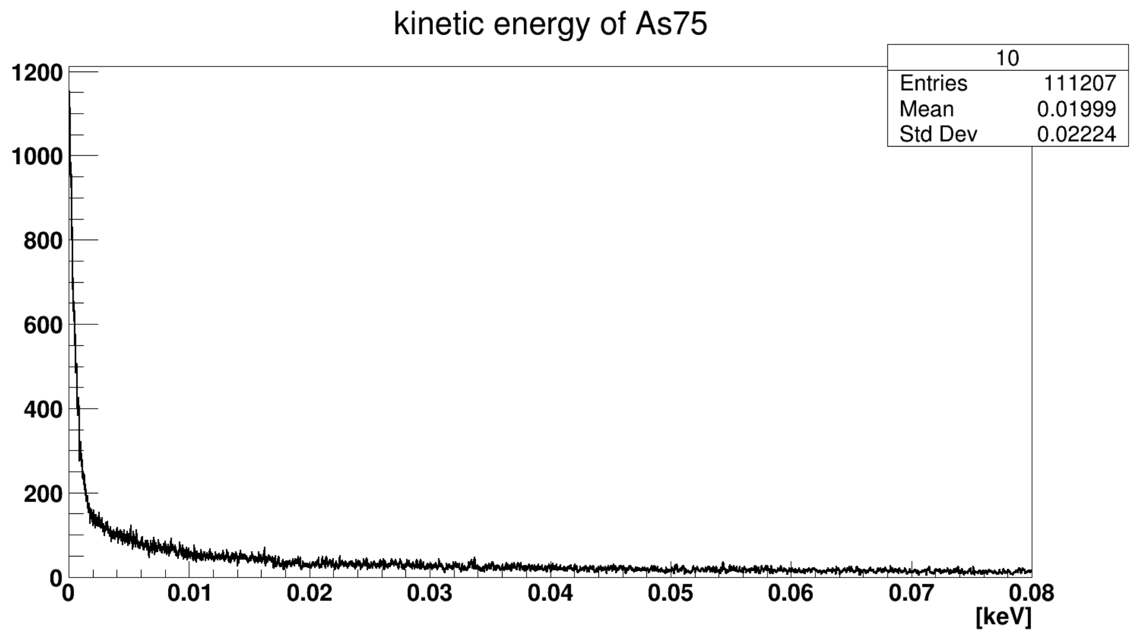


Figure. 3.16. The losses in kinetic energy of As-75 particles when irradiated with a neutron flux spanning a spectrum of energies.

Figure [3.17] illustrates the distribution of different types of reactions. The graph indicates that the number of inelastic and elastic scattering events is comparable to the number of neutron captures events.This is the case because we are dealing with a neutron spectrum that has a distribution of different energies.

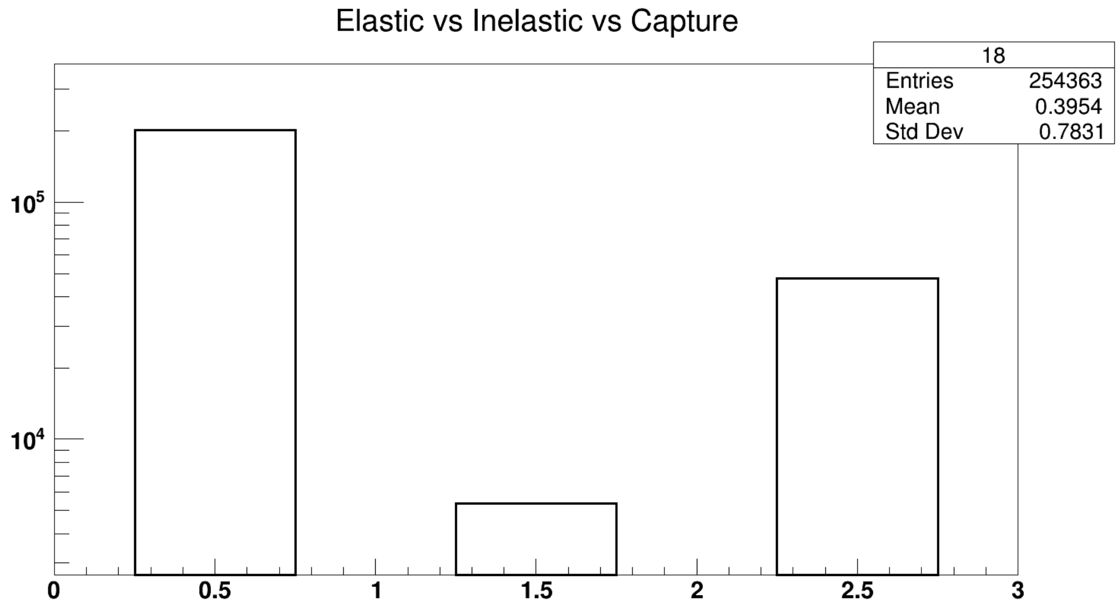


Figure. 3.17. The percentage distribution of reactions as a result of neutron flux spanning a spectrum of energies.

Figure [3.18] illustrates the distribution of secondary particles formed as a result of exposure to high-energy neutron radiation. Indium (In) and arsenic (As) are elements in the semiconductor material, and the defects typically include vacancies or interstitials caused by the displacement of these atoms. Other secondary particles such as alpha particles, protons, and deuterons, while also acting as charge carriers, play significant roles in lattice damage and ionisation, impacting the semiconductor's electronic properties.

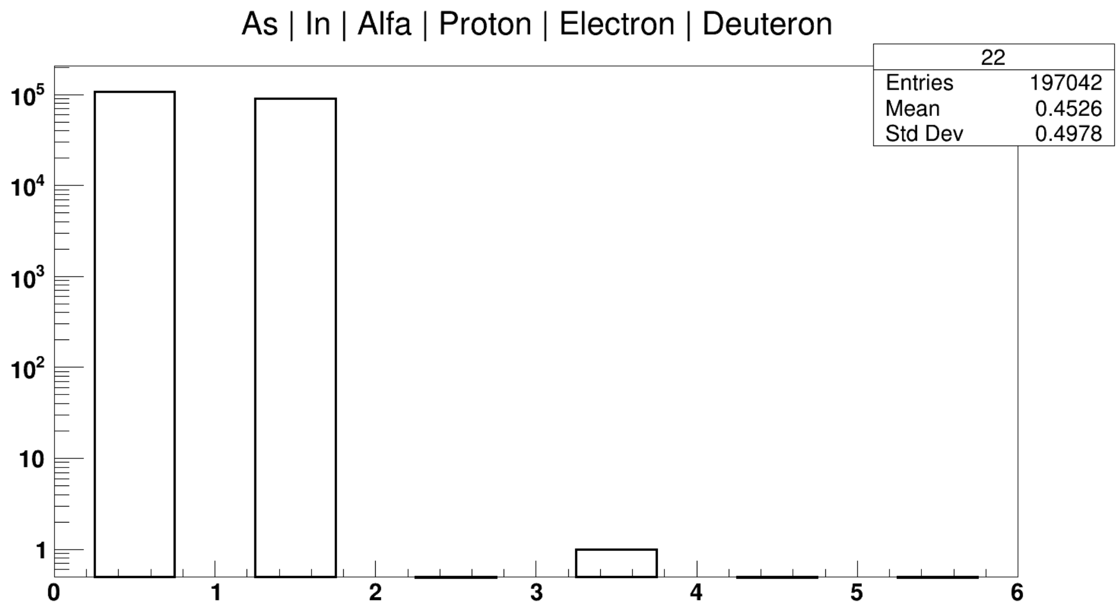


Figure. 3.18. The percentage distribution of secondary particles as a result of neutron flux spanning a spectrum of energies.

Figure [3.19] demonstrates the energy distribution as a result from the neutron capture process. Figure [3.20] demonstrates the energy distribution as a result from the elastic scattering process. Figure [3.18] demonstrates the energy distribution as a result from the inelastic scattering process.

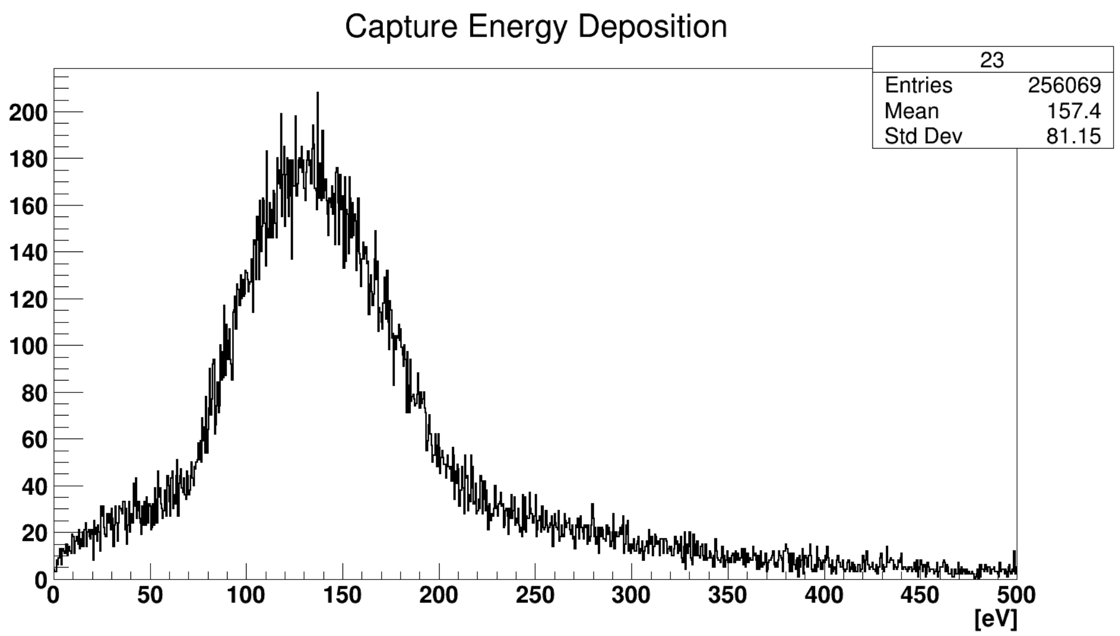


Figure. 3.19. Neutron capture energy deposition

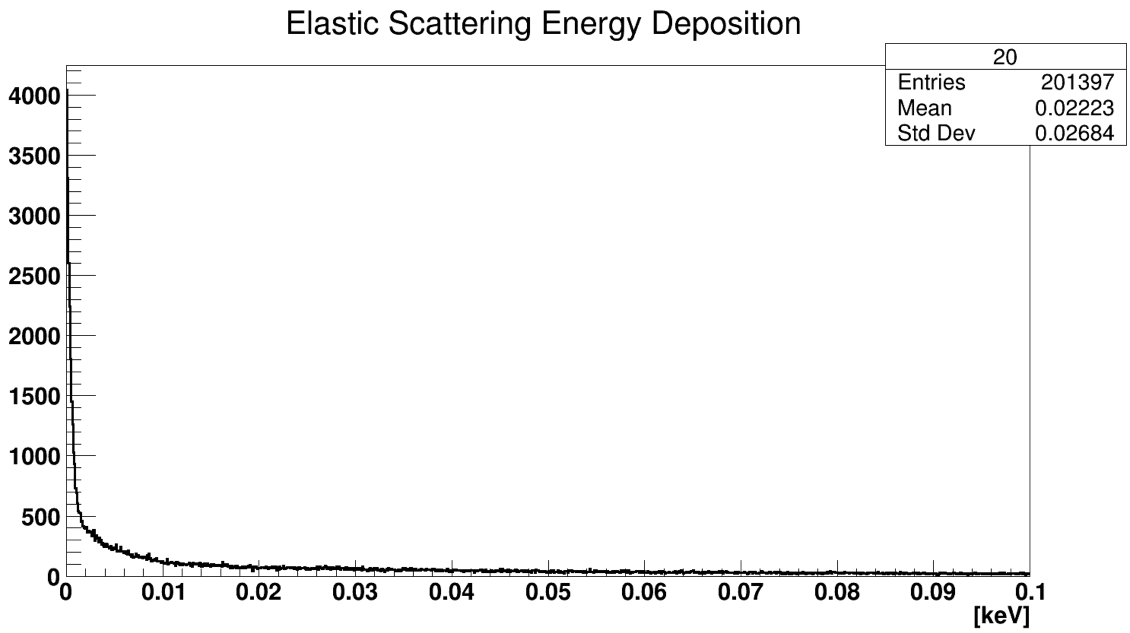


Figure. 3.20. Elastic scattering energy deposition

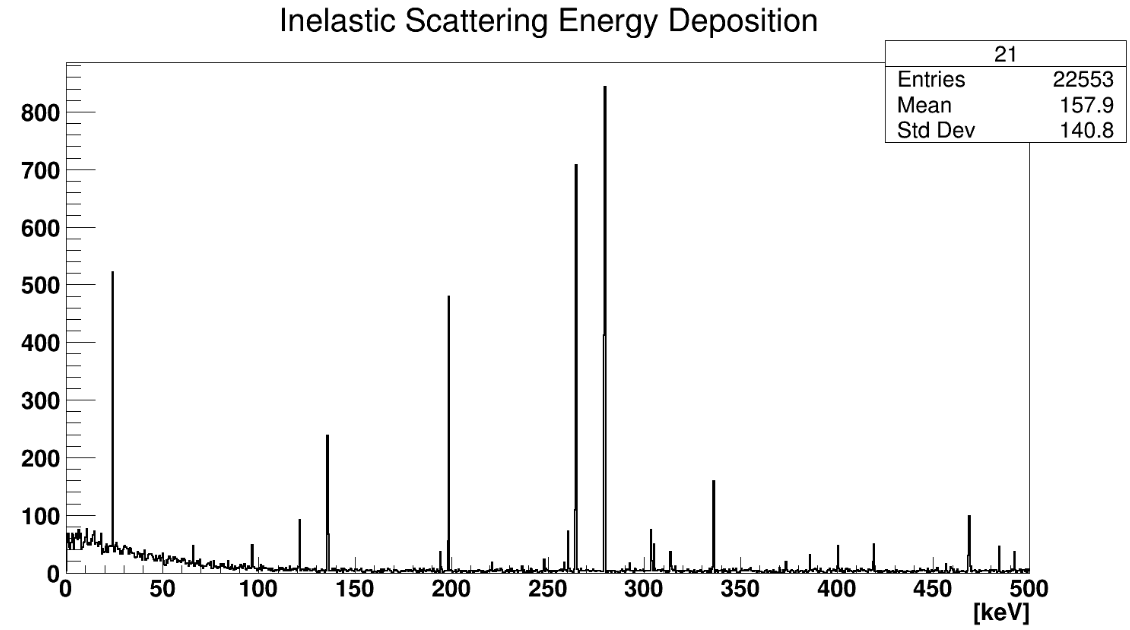


Figure. 3.21. Inelastic scattering energy deposition

CONCLUSION

The analysis of the results indicates a significant dependence of the number of reactions of various types on the energy of the incident neutron in the InAs crystal lattice. In addition, it is important to note the impact of neutron radiation on the crystal lattice of heterostructure semiconductor material. Neutron interaction with the material can cause transient current processes that can lead to errors in device operation, and high current levels can lead to irreversible damage or device destruction. Overall, the analysis results provide a better understanding of the impact of neutron radiation on the material and its potential consequences for devices based on it. The insights gained from this analysis provide a deeper understanding of the mechanisms through which neutron radiation affects heterostructure semiconductor materials. This knowledge is crucial for the design and development of radiation-hardened semiconductor devices. By understanding the specific impacts of different neutron energy levels on the material, engineers and designers can better tailor the materials and structures of devices to mitigate these effects, enhancing the durability and operational stability of devices in radiation-rich environments. The findings not only highlight the susceptibility of these materials to neutron-induced damages but also pave the way for the development of more robust and reliable semiconductor devices. The planned future studies will further enhance this understanding, contributing to the field of semiconductor technology and its application in environments exposed to high levels of radiation.

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