A STUDY AND ANALYSIS OF STOPPING POWER OF DIFFERENT PROJECTILES IN LANTHANIDES AND THEIR COMPOUNDS

A DISSERTATION

SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE AWARD OF THE DEGREE OF

MASTER OF TECHNOLOGY
IN
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SUBMITTED BY

SUKANYA DAS

2K16/NSE/03

UNDER THE SUPERVISION OF

DR. NITIN KUMAR PURI,

ASSISTANT PROFESSOR,

APPLIED PHYSICS DEPARTMENT, DTU

DEPARTMENT OF APPLIED PHYSICS

DELHI TECHNOLOGICAL UNIVERSITY

(FORMERLY DELHI COLLEGE OF ENGINEERING)

BAWANA ROAD, DELHI- 110042

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DELHI TECHNOLOGICAL UNIVERSITY

(Formerly Delhi College of Engineering)

Bawana Road, Delhi-110042

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I, Sukanya Das, Roll No 2K16/NSE/03, student of M.TECH, NUCLEAR SCIENCE AND ENGINEERING, hereby declare that the project dissertation titled "A STUDY AND ANALYSIS OF STOPPING POWER OF DIFFERENT PROJECTILES IN LANTHANIDES AND THEIR COMPOUNDS" which is submitted by me to the Department of Applied Physics, Delhi Technological University, Delhi in partial fulfillment of the requirement for the award of the degree of Master of Technology is original and not copied from any source without proper citation. The work has not previously formed the basis for the award of any Degree, Diploma Associateship, Fellowship or other similar title or recognition.

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DEPARTMENT OF APPLIED PHYSICS

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(Formerly Delhi College of Engineering)

Bawana Road, Delhi-110042

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I hereby certify that the Project Dissertation titled "A STUDY AND ANALYSIS OF STOPPING POWER OF DIFFERENT PROJECTILES IN LANTHANIDES AND THEIR COMPOUNDS" which is submitted by SUKANYA DAS, Roll No. 2K16/NSE/03, Department of Applied Physics, Delhi Technological University, Delhi in partial fulfillment of the requirement for the award of the degree of Master in Technology, is a record of the project work carried out by the student under my supervision. To the best of my knowledge this work has not been submitted in part or full for any Degree or Diploma to this University or elsewhere.

Place: Delhi

Date:

DR. NIITN KUMAR PURI,

ASSISTANT PROFESSOR, SUPERVISOR

DEPARTMENT OF APPLIED PHYSICS, DTU

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SUKANYA DAS

ABSTRACT

A comparative theoretical study of the stopping of different ions and their energy loss in the lanthanide elements and a few of their compounds (mainly oxides and halides) has been presented in this work. The ions that were used to achieve this were the light ion hydrogen, the alkali metal ion lithium, the non-metal ion oxygen, the alkaline earth metal calcium, the transition metals iron and gold, the post transition metal gallium, the metalloid arsenic and the noble gas argon. The values of the stopping were obtained from the software package SRIM-2013 (Stopping and Range of Ions in Matter). The energy of the projectile has been varied from 10keV to 100MeV for the stopping in elements and from 10keV to 10MeV for the stopping in the compounds. The data obtained is rearranged in Microsoft Excel and Origin8 is used for plotting the graphs. An analysis is done for the different kinds of stopping i.e. electronic and nuclear stopping while the ion is traversing through the material. Also their variation along with different parameters is considered. The general inferences drawn from the different plots are mentioned in this work.

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CHAPTER 1

INTRODUCTION

1.1 Interaction of a charged particle inside matter

Whenever a charged particle enters a matter there are various ways it can interact with the matter. But primarily it interacts with coulomb interaction. The interaction occurs in between the positive or negative charge the particle possessing and the negative electrons that are orbiting around the atoms of the medium. However there is chance of interaction with the nucleus but that has a very low probability to occur. A charged particle can execute the following processes while travelling through matter.

- Ionization and excitation of atoms
- Bremsstrahlung
- Cherenkov radiation
- Transition radiation

1.2 Ionization and excitation of atoms

When a positively charged particle enters a medium it interacts with many electrons all at once. The electrons experience coulomb force of attraction when the incoming charged particle passes near them. The interaction causes either excitation or ionization. In case of excitation an electron jumps to a higher orbit within the atom and if it is completely knocked out of its orbit then ionization occurs. The energy the electrons acquire actually comes from the kinetic energy of the particle. As a result the velocity of the incoming charge particle gradually decreases inside the medium. It can be calculated that the maximum energy that a charged particle transfer to a orbital electron is $4Em_o/m$ in a collision. Where m is the mass of the particle, E is the kinetic energy of the particle, and m_o is the mass of the electron.

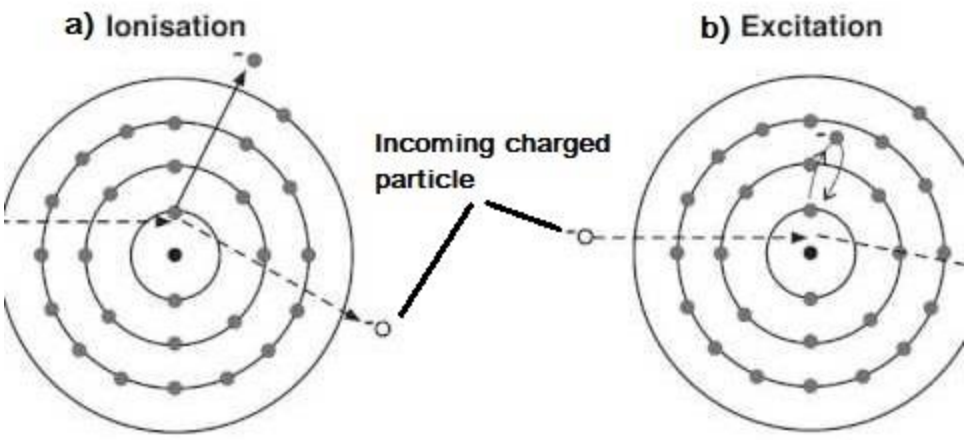


Fig 1.1 Incoming charged particle causing a)ionisation & b)excitation

It can be inferred that a particle losses a very small amount of energy in such a single collision. It is seen that multiple interaction is occurred and the charged particle continuously loses its energy until it is stopped inside the medium. Sometimes after the ionization the freed electrons have some extra energy which they transfer to other electrons to cause further excitation and ionization in the medium. This is an indirect from of transferring energy to the medium from the charged particle. These electrons are called delta electrons. Delta electrons always have a range less than the incoming charged particle.

1.3 Bremsstrahlung

When relativistic particles pass through matter they wiggle due to multiple interactions with the nucleus. This is because they travel almost with the velocity of light which enables them to possess very high kinetic energy with which they can penetrate deeper inside the atom and can go to the vicinity of the nucleus. The nature of this 'collisions' are inelastic.

This interaction accelerates the charged particles. An accelerated charged particle always emits electromagnetic radiation. After being accelerated by the interaction with nucleus the charged particles radiates energy in the form of photons. This radiation is called bremsstrahlung radiation.

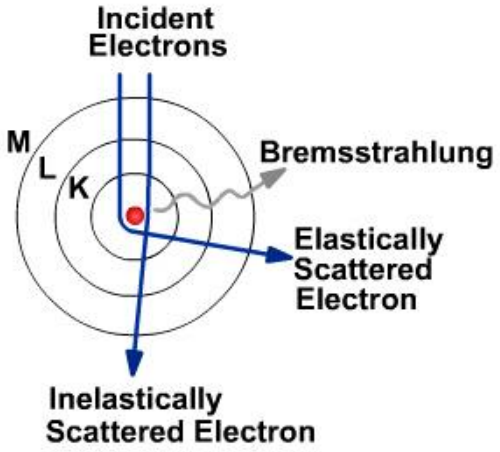


Figure 1.2 schematic diagram of bremsstrahlung radiation

1.4 Cherenkov Radiation

In case of relativistic particles if the particle travels more the velocity of light in that specific homogeneous medium a new type of radiation occurs. This is called Cherenkov radiation. The condition for occurrence of this radiation is the particle velocity v must be greater than c/n where c is the velocity of light and n is the absolute refractive index of the medium. In 1958 Cherenkov was awarded the noble prize along with two other scientists. The emitted light is coherent in nature in an specific direction which can be determined using Huygen's principle.

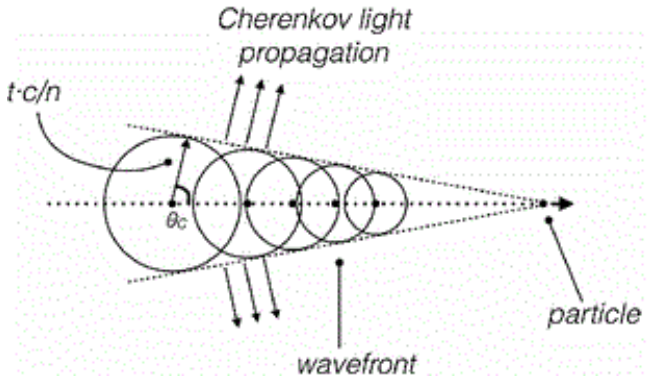


Figure 1.3 schematic diagram of cherenkov radiation

1.5 Transition radiation

When a charged particle passes through the boundary between two materials or an inhomogeneous medium which have different dielectric properties in different regions, transition radiation occurs. The presence of an inhomogeneous medium is the basic difference between transition and Cherenkov radiation. In the part of the material where it has low permittivity the polarization effect becomes smaller and a large extension of the electric field of the moving charge is seen. The portion where the inhomogeneous material has high permittivity the polarization effect becomes larger and a small extension of the electric field of the moving charge is seen.

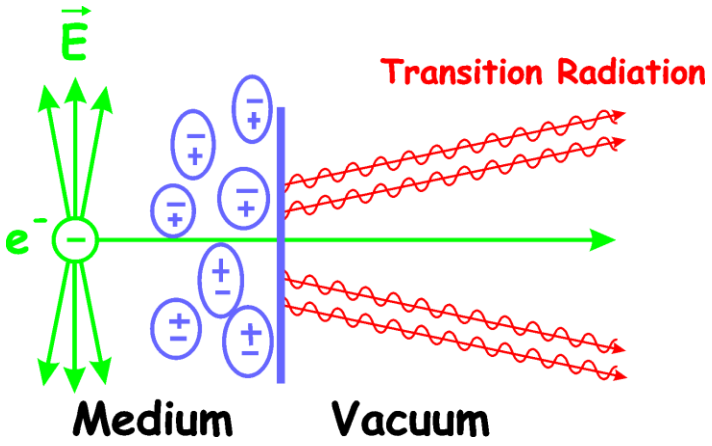


Figure 1.4 Schematic diagram of transition radiation where medium and vacuum is acting as two different medium

1.6 Range of a particle

The range of a particle with specific energy is a unique quantity for a specific medium. During the time the charged particles passage through medium they travel in a straight line path as the coulomb interaction that occurs with the atoms of the medium is not sufficiently strong to deviate them from their path which is a reason that the ionization and excitation of electrons occurs in all direction as a simultaneous process. However when their energy becomes less after many such interactions the velocity becomes minimal and they come in contact with the orbital electrons for a longer period of time it makes them to deviate from their path. Due to this reason at the end of their tracks they do not travel in straight lines anymore. This gives rise to an characteristic property of the charged particle called range. Beyond that length inside the medium the incoming particle cannot pass through.

1.7 Stopping power

Linear stopping power of a charged particle is the ratio of its differential energy loss to the differential path length inside the medium. The following formula gives the mathematical expression of stopping power

$$S = -(dE/dx) \tag{1.1}$$

Where,

S= linear stopping power of the charged particle

dE= differential energy loss inside the medium

dx= corresponding differential length of path

The negative sign implies that the particle loses its energy the further it travels in the medium. The expression (dE/dx) is also termed as the specific energy loss. It tells us about by what rate the particle is losing its energy. For any particle S increases as the velocity of the particle decreases. The Bathe-Bloch formulae express the specific energy loss with great precision. The expression is as follows:

$$-\frac{dE}{dx} = \frac{4\pi e^4 z^2}{m_0 v^2} NB \tag{1.2}$$

Where ,

$$B \equiv Z\left[\ln\frac{2m_0v^2}{I} - \ln\left(1-\frac{v^2}{c^2}\right) - \frac{v^2}{c^2}\right] \tag{1.3}$$

In this expression ,

v= velocity of the incoming charged particle

ze= charge of the incoming charged particle

N= Number density of the absorber medium

Z= atomic number of the absorber medium

e = electronic charge

m_0 = rest mass of the electron

For a non relativistic particle it is seen that B is inversly proportional with the square of the charged particle velocity. It can be explained as, when the particle has higher velocity it spends less time in the vicinity of the electrons and more when it gets slowed down by successive collisions. From equation 1.2 it is also clear that if the particle has more charge the specific energy loss will be higher.

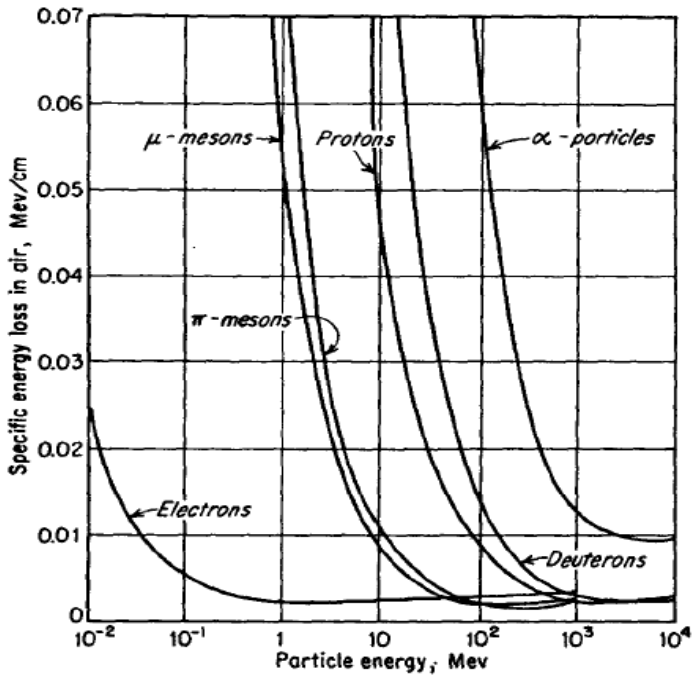


Fig 1.5 The plot of specific energy loss in air vs energy of the charged particle

The product *NZ* represents the electron density of the medium. So material with high atomic number and high density will have greater linear stopping power. From the figure 1.2 it can be

inferred that the energy loss of the charge particle reduces to a certain constant minimal value at higher energies. As the charged particles with higher energy moves with nearly the speed of light, they cause less ionization and hence are termed as “minimum ionizing particles”. Particles like fast electrons also fall in this category.

1.8 Bragg’s curve

The specific energy loss of the charge particle follows a characteristic curve when plotted along its track inside a medium. It is known as Bragg curve. There is an example of such a curve for an alpha particle and beam of alpha particle in fig. 1.3.

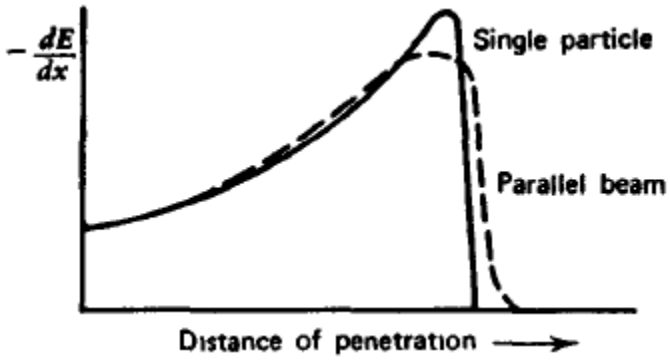


Figure 1.6 Bragg’s curve for alpha particle inside a medium

Whenever a particle passes through a medium the specific energy loss increases in a certain rate that is nearly equal to 1/E upto a certain point. Then it shows a sharp decrease. Most of its energy is lost in the end portion of its track. Reason of this phenomenon is the decrement of the velocity of the incident charged particle gives rise to more interactions where specific energy loss rate is higher.

Inelastic collisions between electrons in the medium and the ion moving through it cause slowing down of the ion. It is termed as inelastic as energy is lost during the process. Electronic stopping power is also considered as momentum transfer between electron gas and ion by some models. An ion experiences large number of collisions with electrons and the charge state of the ion changes frequently while travelling through the medium.

Nuclear stopping power refers to the elastic collisions between the projectile ion and atoms in the sample. The term “nuclear” is meant to note that this type of stopping involves the interaction of the ion with the *nuclei* in the target and it should not be confused with nuclear forces causing stopping. Nuclear stopping increases when the mass of the ion increases. It is larger than electronic stopping at low energy. For very light ions slowing down in heavy materials, the nuclear stopping is weaker than the electronic at all energies.

In the beginning of the slowing-down process at high energies, the ion is slowed down mainly by electronic stopping, and it moves almost in a straight path. When the ion has slowed down sufficiently, the collisions with nuclei (the nuclear stopping) become more and more probable, finally dominating the slowing down. When atoms of the solid receive significant recoil energies when struck by the ion, they will be removed from their lattice positions, and produce a cascade of further collisions in the material. These collision cascades are the main cause of damage production during ion implantation in metals and semiconductors.

When the energies of all atoms in the system have fallen below the threshold displacement energy, the production of new damage ceases, and the concept of nuclear stopping is no longer meaningful. The total amount of energy deposited by the nuclear collisions to atoms in the materials is called the nuclear deposited energy.

1.9 Energy straggling

The microscopic interactions that a charged particle undergoes in a medium is completely random. This random nature makes the energy loss of the charged particle to be a statistical or stochastic process. Due to this if a mono energetic beam of particles pass through a medium a spread in energy occurs. As the distance varies the width of the energy distribution varies. The width of this energy distribution is the measurement of energy straggling.

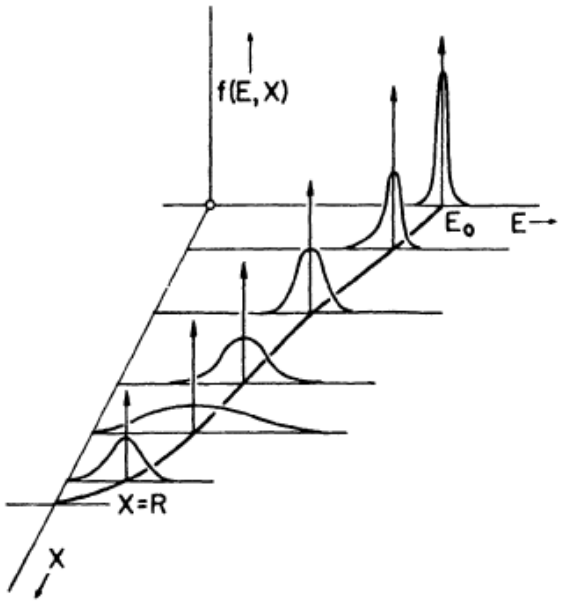


Figure 1.7 plot of an initially mono energetic beam of particles at different penetration length.

In fig.1.4 E represents the energy of the penetrating particles and X is the distance travelled by the beam inside the medium. In the first portion of the plot it can be seen that the distribution gradually becomes more skewed and more wide, which points out the increment of energy straggling as the penetration distance increases. At the end of the track the energy of the particle is greatly reduced, the distribution becomes narrower again.

CHAPTER 2

INTRODUCTION TO LANTHANIDES

2.1 Lanthanides

The lanthanides are a group of 15 elements which are transition metals that are found in the periodic table. The word lanthanide means “like lanthanum” which indicates their chemical properties to be similar to the element lanthanum. The first element of the series has atomic number 57 and the last one has 71.The series starts from lanthanum and ends at lutetium. They can be considered as a subset of the rare earth metals. The lanthanides are:

Lanthanum - atomic number 57 - symbol Ln
Cerium - atomic number 58 - symbol Ce
Praseodymium - atomic number 59 - symbol Pr
Neodymium - atomic number 60 - symbol Nd
Promethium - atomic number 61 - symbol Pm
Samarium - atomic number 62 - symbol Sm
Europium - atomic number 63 - symbol Eu
Gadolinium - atomic number 64 - symbol Gd
Terbium - atomic number 65 - symbol Tb
Dysprosium - atomic number 66 - symbol Dy
Holmium - atomic number 67 - symbol Ho
Erbium - atomic number 68 - symbol Er
Thulium - atomic number 69 - symbol Tm
Ytterbium - atomic number 70 - symbol Yb
Lutetium - atomic number 71 - symbol Lu

The 4f electron shell is gradually filled in this group. All but one of them are f-block elements. Sometimes lutetium is excluded from the group as it has a single valence electron in the 5d shell.

Lanthanum	Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium	Terbium	Dysprosium	Holmium	Erbium	Thulium	Ytterbium	Lutetium
57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm [145]	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.05	71 Lu 174.97

Primordial | From decay | Synthetic **Border** shows natural occurrence of the element

.

2.2 Physical and chemical properties of lanthanides

- As lanthanides are transitional metals they have metallic characteristics. In pure form they have bright metallic luster which makes them silvery in appearance.
- Lanthanides are soft metals, like sodium they can be cut using a knife.
- Lanthanides generally form trivalent cations and hence considered to have +3 oxidation state. In early years of research it was found that samarium, europium and ytterbium forms +2 oxidation states in a solution. But further research has confirm that all of the element in this series can form +2 or +4 stable oxidation states in solution under different condition.
- They do not occur free in nature.
- Lanthanide ions show luminescent properties as they have unique 4f orbitals.
- The trivalent ions formed by lanthanides with an exception of lanthanum and lutetium, have unpaired f electrons. Even though the magnetic moments of them deviate greatly from spin only values. This is because they possess strong spin-orbit coupling.
- If we move from left to right in the periodic table then the radius of the lanthanides gradually decreases. This is due to the increase in positive charge of the nucleus. This phenomenon is called lanthanide contraction.
- The metal aluminum has comparable ionization energies with the lanthanides. For aluminum first three ionization energies is summed as 5139 $kJ \cdot mol^{-1}$. The sum of the three ionization energies of lanthanides fall in the range of 3455 – 4186 $kJ \cdot mol^{-1}$.
- They are reactive and have a tendency to form ionic compounds reacting readily with other elements.
- Cerium, praseodymium, neodymium, lanthanum and europium reacts with oxygen in the air even if they are exposed for a very brief period of time.

2.3 Storage of lanthanides:

Lanthanides are highly reactive in nature. Due to this they have to be stored in such a environment where they won't be able to react readily. They are generally stored in a container filled with inert gas like neon or argon. Keeping them under mineral oils also separates them from the atmosphere.

2.4 Compounds of lanthanides

Ln(III) compounds

As lanthanides form trivalent ions they tend to form ionic compounds with other elements. Between oxygen donor ligands and nitrogen donor ligands lanthanides form more stable complexes with the former. In aqueous solutions the ether 9 or 8 coordinates. But the smaller 8-coordinate $[Ln(H_2O)_8]^{3+}$ has more water molecule in second coordination sphere. Monodentate ligands is weak as displacement of water from primary of first coordination sphere. Hence due to chelate effect, chelating ligands are formed.

Ln(II) and Ln(IV) compounds

Divalent halide derivatives are formed by the lanthanides. Some of them are conventional salts and some are Ln(III) "electride"-like salts. YbI_2, EuI_2, and SmI_2 are the examples of conventional salts formed by lanthanides. LaI_2, CeI_2 and GdI_2 are the examples of electride-like salts .The iodies of lanthanides are mostly soluble in ethers. This includes $TmI_2(dimethoxyethane)_3$. Among the iodides Samarium(II) iodide is used as reducing agent.

Transmetalation reactions can form Ln(II) complexes... Tetravalent lanthanides are generally rare. The Ce(IV) is the only exception due to its tendency to form an unfilled f shell and hence can be used as oxidizing agent.

Hydrides

The reaction of lanthanide metals with hydrogen to from hydrides is through exothermal reactions. The general formula by which lanthanides hydrides can be expressed is LnH_x. All the dihydride compounds formed by lanthanides are black pyrophoric and good conductors. But Eu

and Yb dihydrides are transparent and salt like. In the face centred lattice unit cell structure of such dihydrides hydrogen atoms occupy the tetrahedral sites.

Non-stoichiometric trihydrides can be produced by further hydrogenation of the dihydrides. These trihydrides are salt like, more anionic in character and non conducting in nature.

Halides

The lanthanides are trivalent and hence generally form trihalide compounds reacting with fluorine, chlorine, bromine and iodine . They are ionic in nature, have high melting point and are sensitive to air (except trifluorides). They are soluble in water and forms oxohalides in high temperature reactions. Pure metals or lanthanides can be extracted from trihalides.

Tetrahalides are very rare to form however tetrafluorides of cerium, praseodymium, terbium, neodymium and dysprosium has been reported which are produced in special conditions.

The dihalides are divides into two parts, some are conducting and the rest are insulators.

Lanthanides can form only one monohalide that is LaI which is produced from La triiodide.

Carbides

Lanthanides form carbides of varying stoichiometry. The dicarbides are metallic conductors (exception EuC_2) with the structure like calcium carbide. However the single bond between the carbons is longer in case of lanthanide carbides. They undergo hydrolysis and produce mixture of hydrocarbons along with hydrogen gas.

Borides

All the lanthanides reacts with boron and form borides . the general formulae can be written as LnB_x. The borides which are relatively bulky and contain more than 12 boron atoms show semi conductivity.

Diborides (LnB_2) are formed by Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu. They all have a graphitic layer of boron atoms. They show ferromagnetic transitions in low temperature.

Tetraborides (LnB_4) are formed by all of the lanthanides except EuB_4. Their structure consists of a boron sub-lattice with chains of octahedral B_6 clusters which are linked by boron atoms. They are good conductors and antiferromagnetic in nature.

Hexaborides (LnB_6)is formed by all of the lanthanides. They have cation defect which makes them to be non-stoichiometric. EuB_6 shows semiconductivity & the others are good conductors. Dodecaborides(LnB_{12}) are formed by the heavier lanthanides which are smaller in size, but not by, La – Eu as they are larger in size and lighter. However there is an exception $YbB_{12.}$

Even borides like LnB_{66} is also formed by for all lanthanide metals. These compounds are known to be non-stoichiometric. They have a very complex structure having 1600 atom containing unit cells.

Organometallic compounds

With carbon atom lanthanides form stable σ bonds. As the 4f orbital is buried deep in the atom, the electrons of this orbital do not form orbital overlap in the exterior region of the atom. This makes lanthanides to show ionic character. The lanthanides have large size and because of this they form stable organometallic compounds with ligands which are bulky. Example of such a compound is $Ln[CH(SiMe_3)_3]$.

2.5 Uses of lanthanides

- The first red phosphor which was used in cathode ray tubes to invent color television was europium-doped yttrium vanadate.
- Because of forbidden f-f transitions in case of lanthanides the decay of an excited electron to its ground state is slow which gives rise to metastable states and makes them suitable candidates to produce laser. Hence in widely used Nd:YAG laser population inversion is easily achieved.
- In optical spectrometers holonium oxide containing glass is used as it shows sharp optical absorption peaks in 200-900 Nano meter spectral range.
- They are used to make superconductors.
- Neodymium-iron-boron is used to make rare earth magnets with high flux .
- They are used in electronic polishers.

- Lanthanides are used as refining catalyst in hybrid car batteries.
- LaB_6 and CeB_6 shows thermionic emission and used in scanning electron microscopes.
- In optical fiber based communication erbium doped fiber is used.
- To produce microwave resonators, yttrium iron garnet is used widely.
- In tungsten iron garnet based welding lanthanide oxides are added with tungsten. This improves the high temperature properties.
- It is also used in defense technologies like night vision goggles and range finders.
- Gd^{3+} has the maximum number of unpaired electrons among all lanthanide ions. The number of unpaired electrons is 7. The magnetic moment is experimentally calculated to be 7.94 Bohr magneton. The unpaired electrons of Gd3+ have parallel spins which makes it very suitable in MRI scans as contrast reagent.

CHAPTER 3

SOFTWARES USED

Stopping and Range of Ions in Matter (**SRIM**) is a group of computer programs developed by James F. Ziegler and Jochen P. Biersack around 1983. These programs simulate the interaction of ions with matter. SRIM is widely used in the technology community, especially in the research of ion implantation and also in branches of radiation material science.

Applications of SRIM include:

- Ion Stopping and Range in Targets: SRIM does calculations which results in tables of stopping powers, range and straggling distributions for any ion at any energy in any elemental target.
- Ion Implantation: The SRIM package can be used to simulate ion beams that are used to modify samples by injecting atoms to change the target chemical and electronic properties. The damage caused to solid targets by atom displacement and other kinetic effects associated with the physics of this kind are also taken into consideration.
- Sputtering: The process of knocking out target atoms is called sputtering. The calculation of sputtering can also be done by the SRIM package.
- Ion Transmission: Ion beams can be followed through mixed gas/solid target layers, such as occurs in ionization chambers or in energy degrader blocks used to reduce ion beam energies.
- Ion Beam Therapy: Ion beams are widely used in medical therapy, especially in radiation oncolog**y.**

SRIM was originally developed as a DOS program called TRIM in 1980. Since then the programs are being continuously upgraded with the changes that occur approximately after every five years. A Monte Carlo simulation method, namely the binary collision approximation forms the basis of SRIM. The binary collision approximation (BCA) is a method, widely used in ion irradiation physics, which efficiently enables computer simulation of the penetration depth and defect production by energetic (with kinetic energies in the kilo-electron volt (keV) range or higher) ions in solids. In this method, the ion is roughly assumed to travel through a material by

experiencing sequential independent binary collisions with sample atoms (nuclei). Between the collisions, the ion experiences electronic stopping power and is approximated to travel in a straight path. The classical scattering integral between two colliding particles is solved to analyze a single collision between the incoming ion and a target atom (nucleus) for the impact parameter of the incoming ion. Solution of the integral gives the scattering angle of the ion and its energy loss to the sample atoms, and hence the energy is after the collision as compared to before it can be calculated. The time has elapsed during the collision can also be calculated by solving the time integral of the collision. The energy loss to electrons, i.e. electronic stopping power, can be treated either with impact-parameter dependent electronic stopping models or by subtracting a stopping power dependent on the ion velocity only between the collisions, or a combination of the two approaches. SRIM is the most widely used BCA code now. It offers a GUI and it can be used to simulate linear collision cascades for all ions in all materials up to ion energies of 2 GeV.

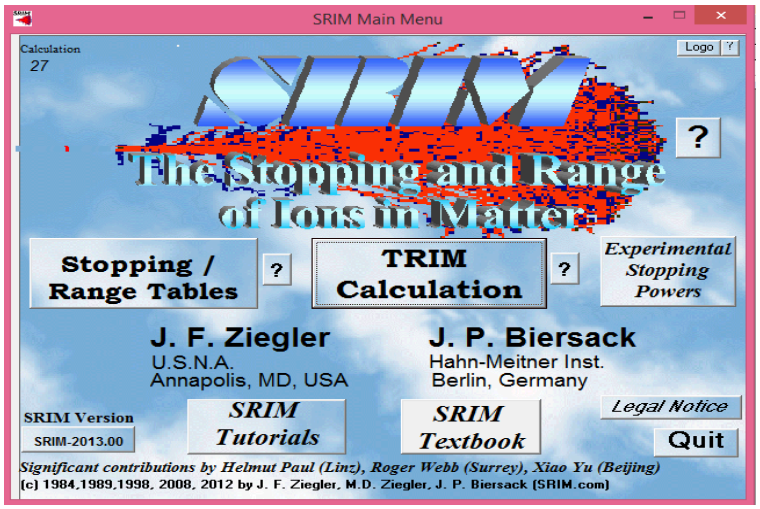
SRIM takes the ion type and energy (between the range 10eV – 2 GeV) as the input. A button labeled as PT lists all the elements in the periodic table that can be used as the incident ion. It also takes the material of target element as input. There can be also multiple target elements. The same PT button can be used to add different elements to the target. For compounds the relative stoichiometry of each element in the compound should be entered. In addition there is also a compound dictionary which categorizes different compounds into nuclear physics materials, common target materials, metal alloys, plastics and polymers, biological compounds, liquids and gases among others. There is also a provision to change the density of the target in case it is not accurately calculated by the program and to determine if the material is gaseous. It takes only homogenous targets in this calculation and layered structures are not allowed. It lists the 3D distribution of the ions in the solid and its parameters, such as penetration depth, its spread along the ion beam (called straggling) and perpendicular to it and energy partitioning between the nuclear and electron losses as the output. SRIM has an easy-to-use user interface and built-in default parameters for all ions and materials. These features have made SRIM immensely popular. However, the crystal structure or the dynamic composition changes in the material are not taken into account that causes limitations in its efficiency. The influence of neighboring atoms, the description of ion channeling effects, recombination of knocked off atoms (interstitials) with the vacancies are some parameters which are neglected. Also defect clustering

and irradiation-induced amorphisation are not defined, even though they are very important in most materials especially semiconductors. A large number of experiments are averaged to determine the electronic stopping power.

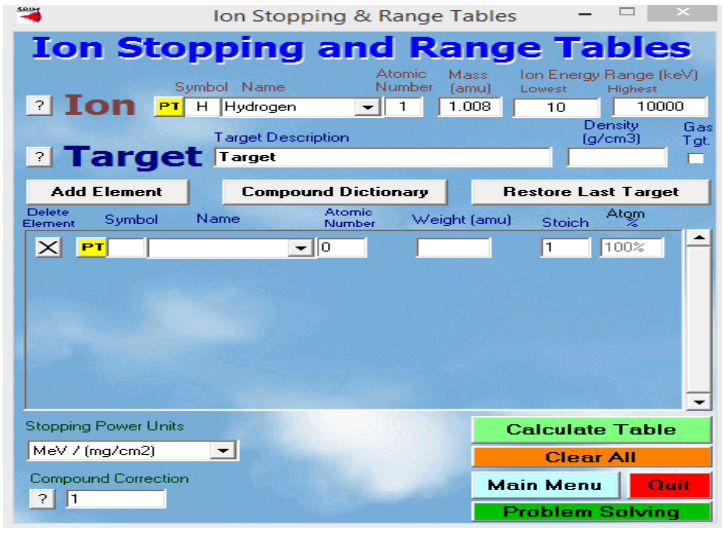
Using SRIM

This section covers how to determine the stopping and range tables for any combination of ion and target elements/compounds.

- The SRIM icon on the desktop is opened. The main menu of SRIM appears.



- **Stopping and Range Tables** (S & R Tables) is selected from the main menu. The following window appears.



- First the ion is entered. The PT button can be used to view the entire periodic table to select an ion of any choice.
- SRIM will automatically enter the various boxes describing the ion.
- The energy range can be entered according to required specifications.
- Then the target is specified. The program again automatically enters various boxes describing the target.
- The term "Stoich" is used for compound targets, for the stoichiometry of each of the elements of the compound.
- The density of compound targets can be varied accordingly as a prompt appears asking to consider the density.
- Calculate Table is clicked**.**
- The suggested filename, for example "*SRIM Outputs\Arsenic in Silicon*" is accepted. This file is stored in the SRIM directory: *../SRIM Outputs/* if needed to be referenced again.
- A table with different parameters appear.

```
==================================================
          SRIM version ---> SRIM-2013.00
          Calc. date   ---> July 26, 2018
==================================================

Disk File Name = SRIM Outputs\Arsenic in Silicon.txt

Ion = Arsenic [33] , Mass = 74.92 amu

Target Density =  2.3212E+00 g/cm3 = 4.9770E+22 atoms/cm3
======= Target  Composition ========
  Atom   Atom   Atomic    Mass
  Name   Numb   Percent   Percent
  ----   ----   -------   -------
   Si     14    100.00    100.00
====================================
Bragg Correction = 0.00%
Stopping Units =  MeV / (mg/cm2)
See bottom of Table for other Stopping units

     Ion        dE/dx      dE/dx     Projected  Longitudinal   Lateral
    Energy      Elec.      Nuclear     Range     Straggling   Straggling
 ------------  ---------- ---------- ----------  ----------
 10.00 keV  2.751E-01 4.062E+00    124 A       47 A        35 A
 11.00 keV  2.886E-01 4.159E+00    131 A       49 A        37 A
 12.00 keV  3.014E-01 4.245E+00    139 A       51 A        39 A
 13.00 keV  3.137E-01 4.323E+00    146 A       54 A        41 A
 14.00 keV  3.255E-01 4.394E+00    154 A       56 A        43 A
 15.00 keV  3.370E-01 4.458E+00    161 A       58 A        45 A
 16.00 keV  3.480E-01 4.518E+00    168 A       60 A        46 A
 17.00 keV  3.587E-01 4.572E+00    175 A       63 A        48 A
 18.00 keV  3.691E-01 4.622E+00    182 A       65 A        50 A
 20.00 keV  3.891E-01 4.711E+00    196 A       69 A        53 A
 22.50 keV  4.127E-01 4.805E+00    213 A       74 A        57 A
```

- This table can be used in other spreadsheet application like Microsoft Excel to analyze the data. The data available in the table are upto the energy range that was entered earlier.

ORIGIN

Origin is a computer program produced by OriginLab Corporation for interactive scientific graphing and data analysis. It runs on Microsoft Windows and supports graphing in various 2D/3D plot types. Statistics, signal processing, curve fitting and peak analysis are some data analyses that are included in origin. Origin was originally created for the sole use with microcalorimeters manufactured by MicroCal Inc. Graphing of the instruments data, performing nonlinear curve fitting and parameter calculation was done by the software.

In 1992 Microcal Software first made the software available to the public. Microcal Software was later was renamed to OriginLab Corporation, located in Northampton, Massachusetts.

Origin supports the import of data files in various formats such as ASCII text, Excel, NI TDM, DIADem, NetCDF, SPC, etc. It can also export the graph to various image file formats such as JPEG, GIF, EPS, TIFF, etc. Origin is a primarily GUI software with a spreadsheet front end. However unlike popular spreadsheets like Excel, Origin's worksheet is column oriented. Unlike the cell formula that is used in excel, calculations are done using column formula in Origin. Each column has associated attributes like name, units and other user definable labels. The user relies on customizable graph templates, analysis dialog box Themes which save a particular suite of operations, auto recalculation on changes to data or analysis parameters, and Analysis Templates™ which save a collection of operations within the workbook.

Origin is available in two editions, the regular version Origin and OriginPro. The latter adds additional data analysis features like surface fitting, short-time Fourier Transform, and more advanced statistics.

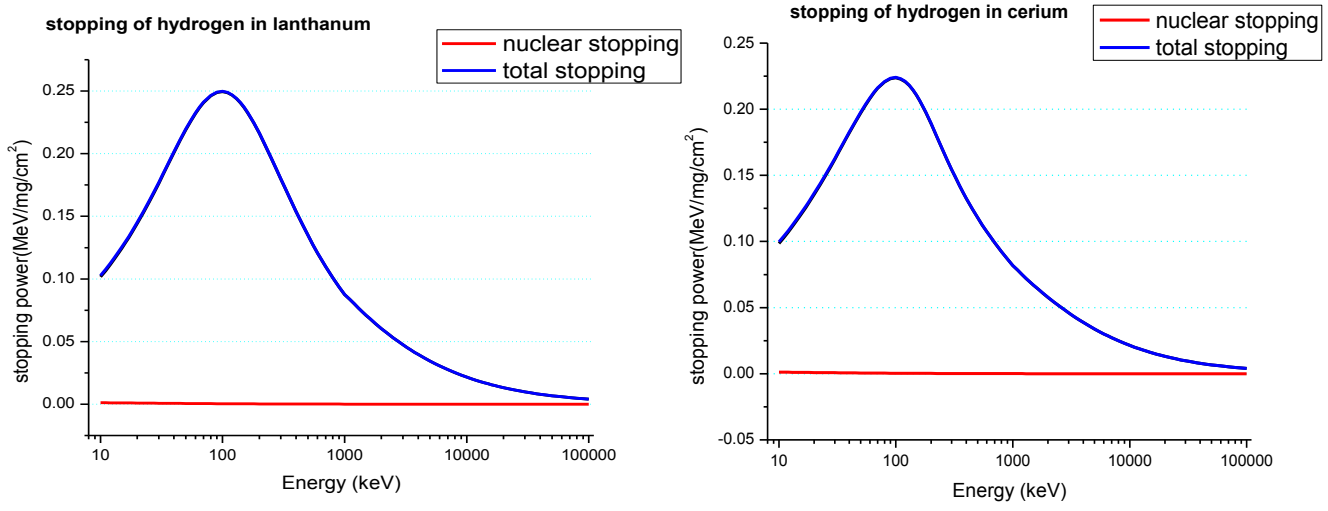
CHAPTER 4

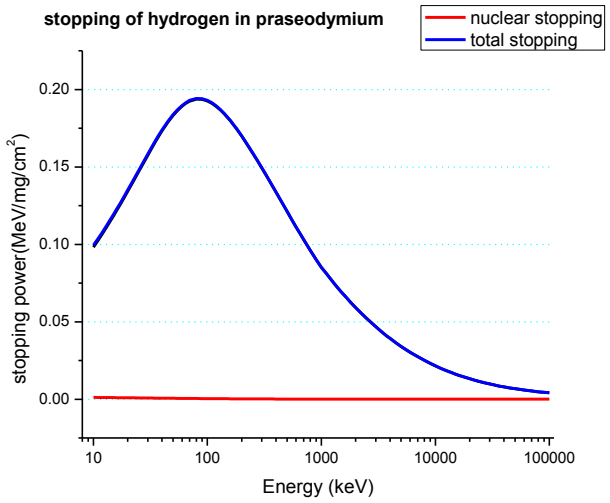
RESULTS AND DISCUSSIONS

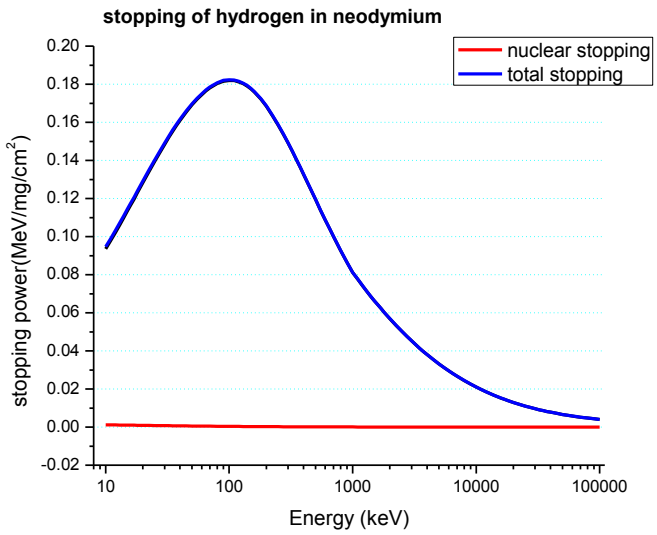
An analysis of the stopping power in the 15 lanthanide elements (ranging from atomic numbers 57 -71) and their compounds due to different incident projectiles has been presented in this work. The ions that are used to achieve this are Hydrogen (Z=1), Lithium (Z=3), Oxygen (Z=8), Argon (Z=18), Calcium (Z=20), Iron (Z=26), Gallium (Z=31), Arsenic (Z=33) and Gold (Z=79). The range tables were calculated using SRIM software package. The interaction of each of these ions with all the lanthanides has been discussed. For the lanthanide elements the energy range has been taken from 10kev to 100MeV. For the compounds the energy range has been taken from 10kev to 10MeV. The range tables are referenced from the Outputs folder of SRIM and then the data is rearranged in excel sheets before using the data in Origin for plotting. The plots obtained from Origin8 are analyzed carefully and the following inferences are drawn.

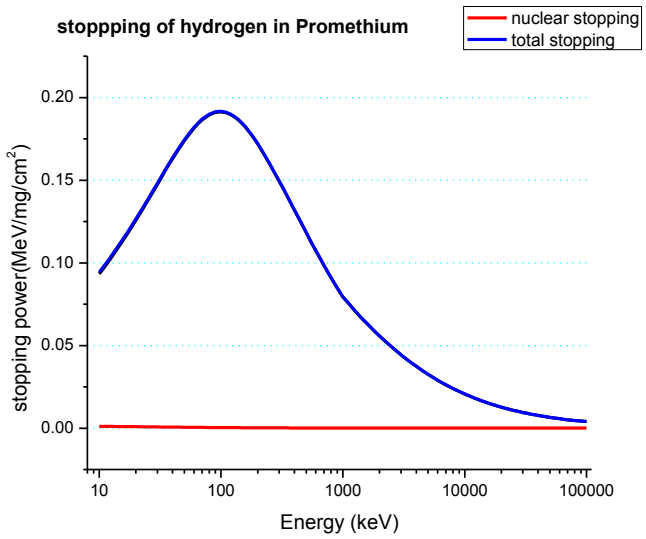
Stopping of Hydrogen in the Lanthanide elements

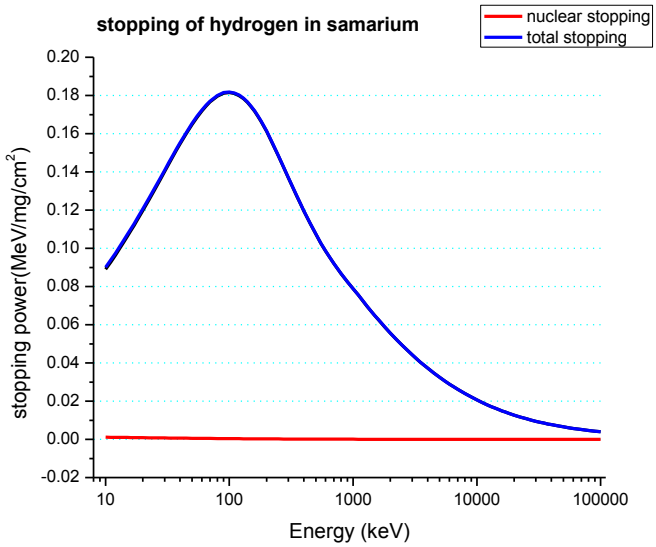
The following plots were obtained for stopping of hydrogen ion in lanthanide elements.

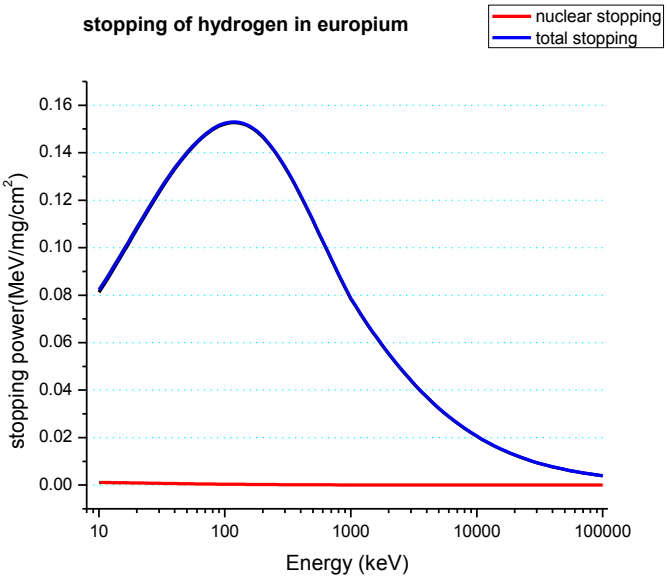


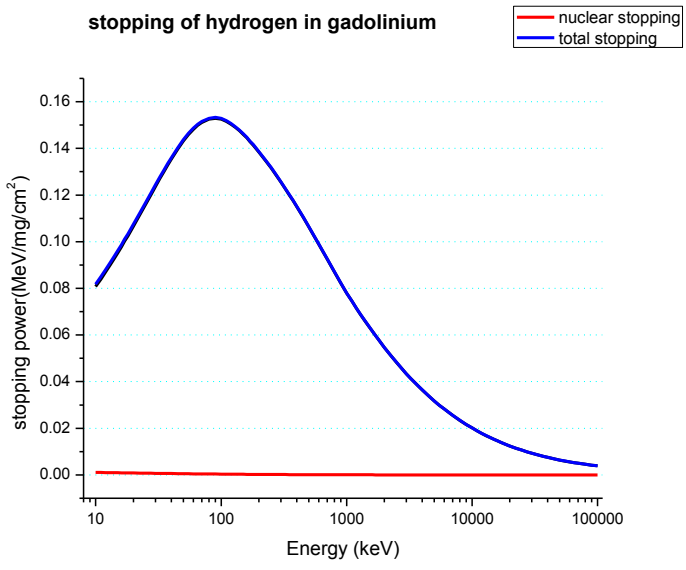

stopping of hydrogen in praseodymium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.20
0.15
0.10
0.05
0.00
10
100
1000
10000
100000
Energy (keV)

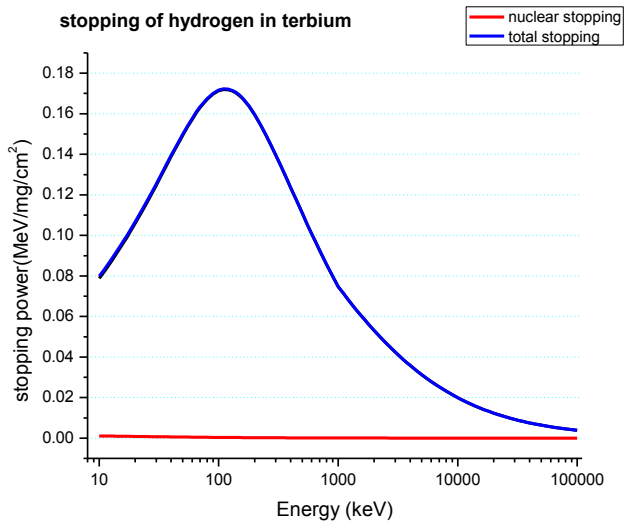

stopping of hydrogen in neodymium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
10
100
1000
10000
100000
Energy (keV)

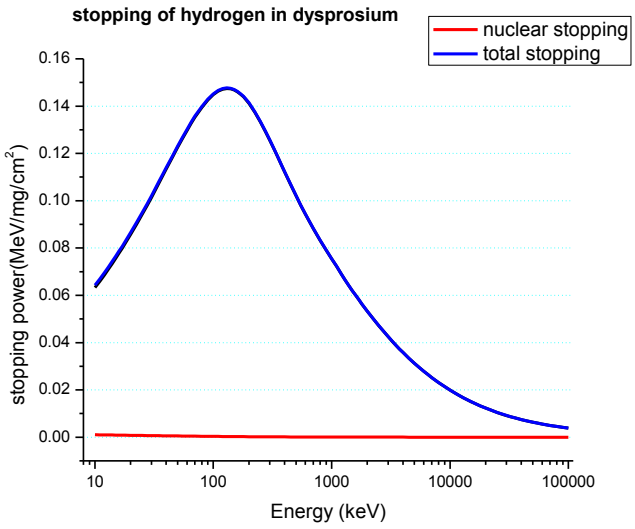

stoppping of hydrogen in Promethium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.20
0.15
0.10
0.05
0.00
10
100
1000
10000
100000
Energy (keV)

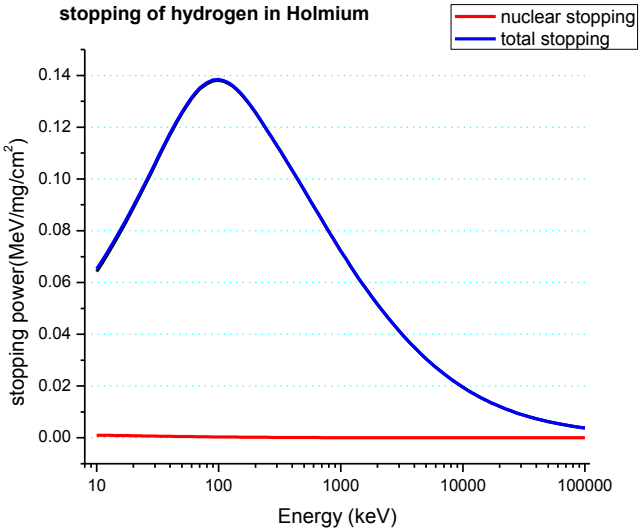

stopping of hydrogen in samarium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
10
100
1000
10000
100000
Energy (keV)

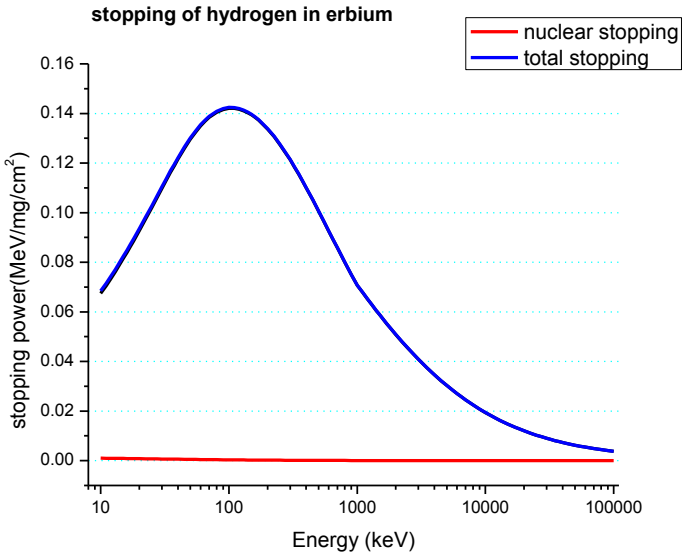

stopping of hydrogen in europium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
10
100
1000
10000
100000
Energy (keV)

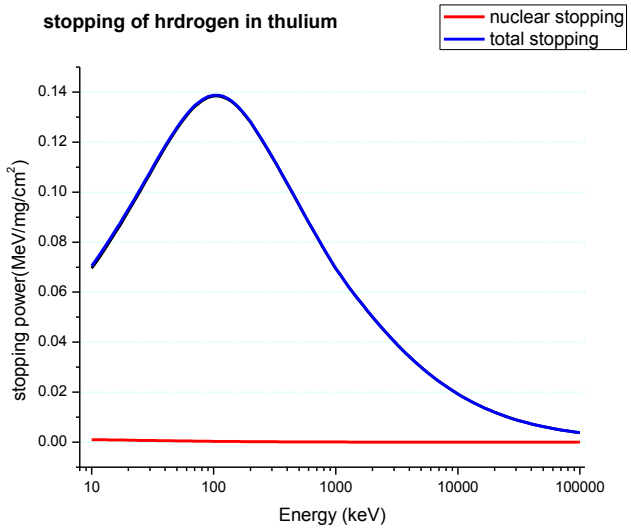

stopping of hydrogen in gadolinium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
10
100
1000
10000
100000
Energy (keV)

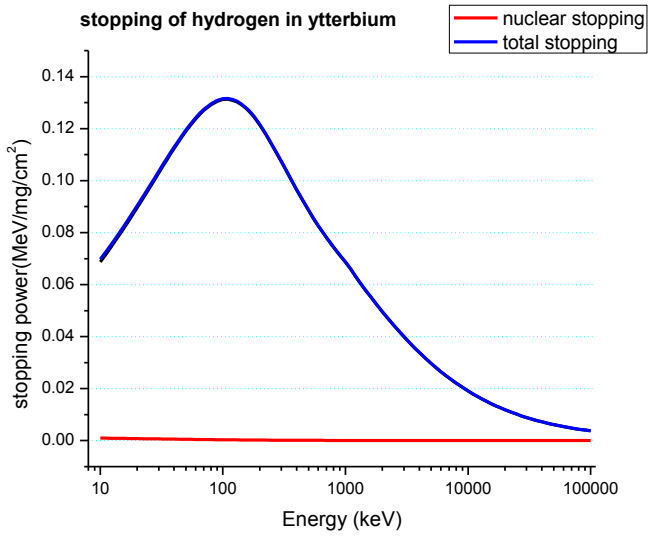

stopping of hydrogen in terbium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
10
100
1000
10000
100000
Energy (keV)


stopping of hydrogen in dysprosium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
10
100
1000
10000
100000
Energy (keV)


stopping of hydrogen in Holmium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
10
100
1000
10000
100000
Energy (keV)


stopping of hydrogen in erbium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
10
100
1000
10000
100000
Energy (keV)


stopping of hrdrogen in thulium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
10
100
1000
10000
100000
Energy (keV)


stopping of hydrogen in ytterbium
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
10
100
1000
10000
100000
Energy (keV)

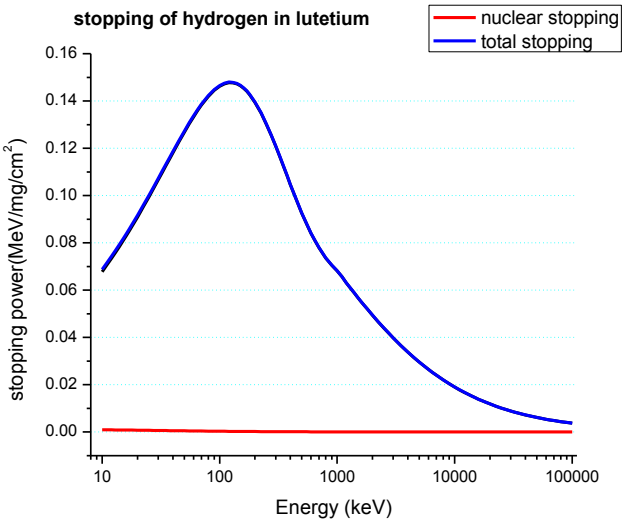
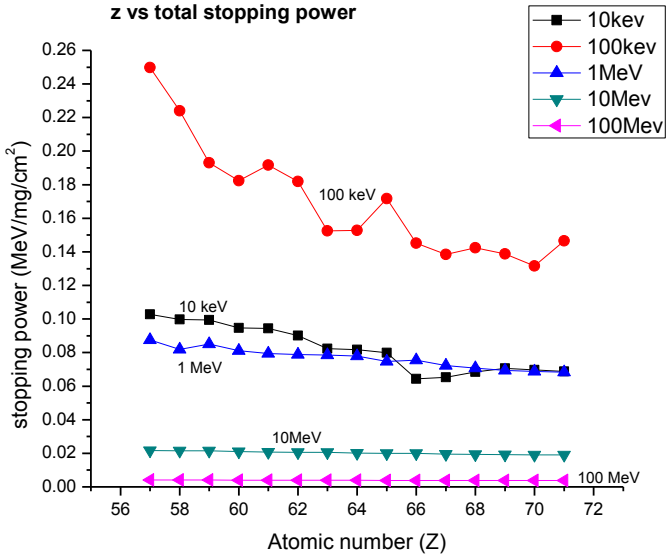


Fig4.1: Stopping of hydrogen in different lanthanide elements

The electronic stopping is almost equal to the total stopping with very less contribution from nuclear stopping to the total stopping. The electronic stopping power gradually increases till approximately 100KeV and gradually decreases after. Nuclear stopping always remain less than electronic stopping. The stopping at lower energies is higher than of those at higher energies. With increase in the atomic number of the target, the maximum stopping i.e. the peak lowers. Also the starting point i.e. the stopping at 10keV lowers from 0.1 MeV/mg/cm^2 to about 0.06 MeV/mg/cm^2. Also from the following plots we can see that both the electronic stopping and nuclear stopping decrease with increase in atomic number of the target.



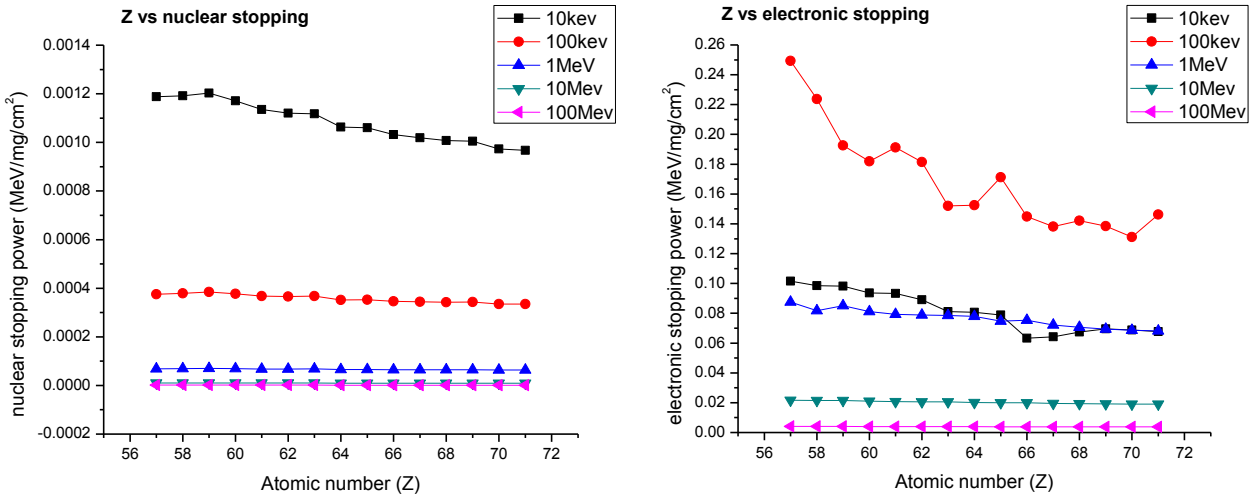
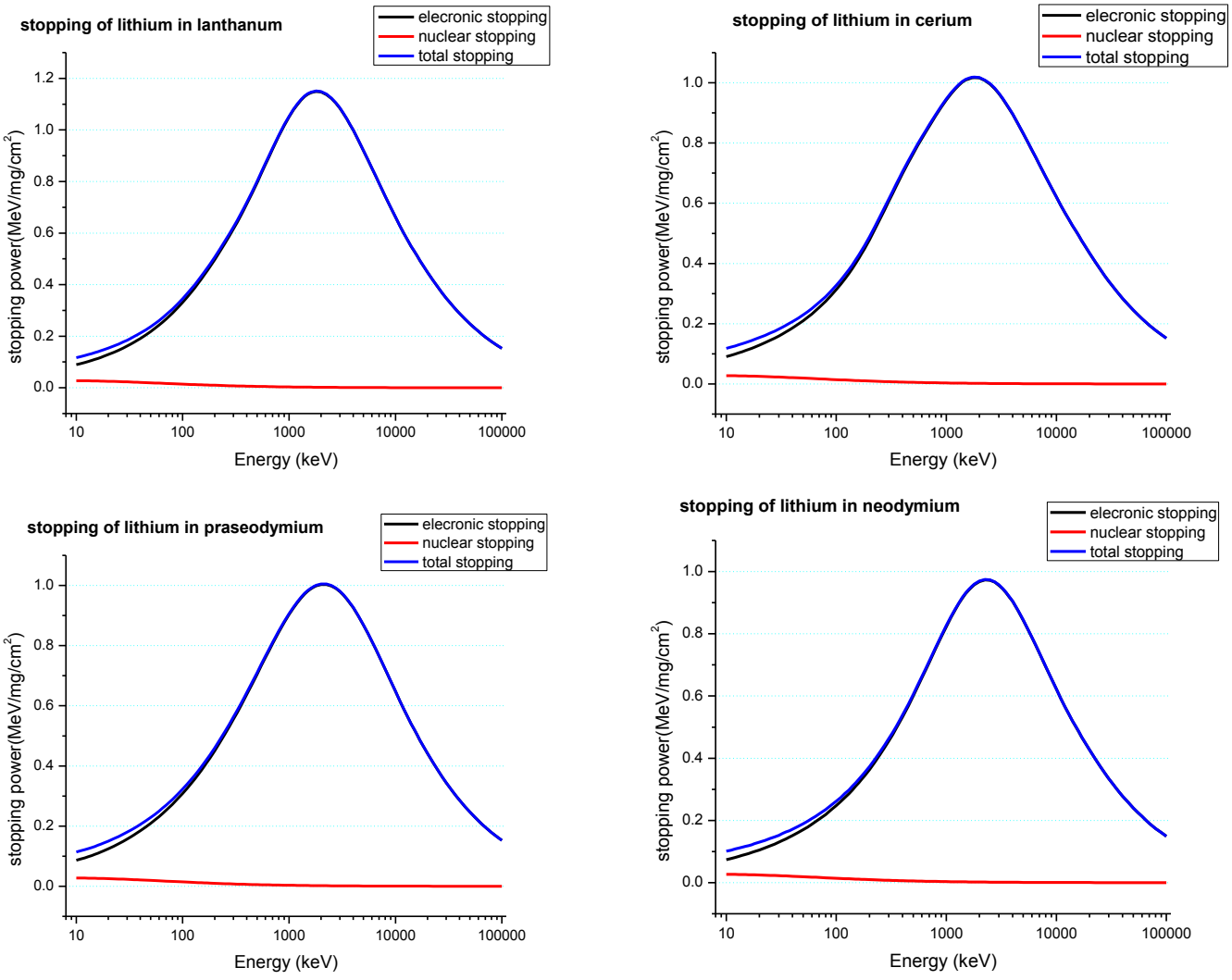
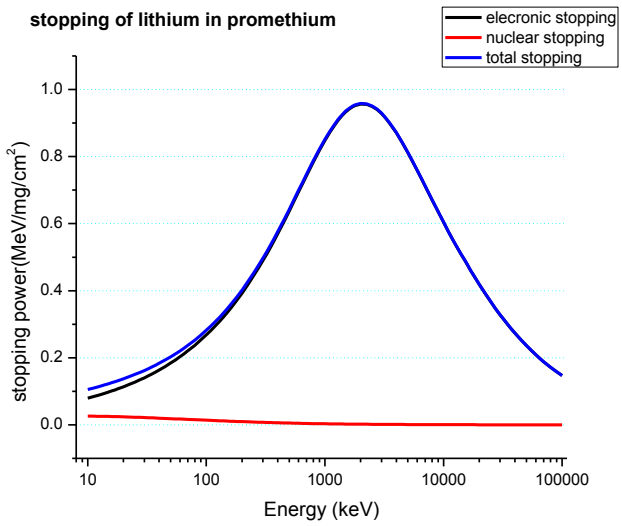


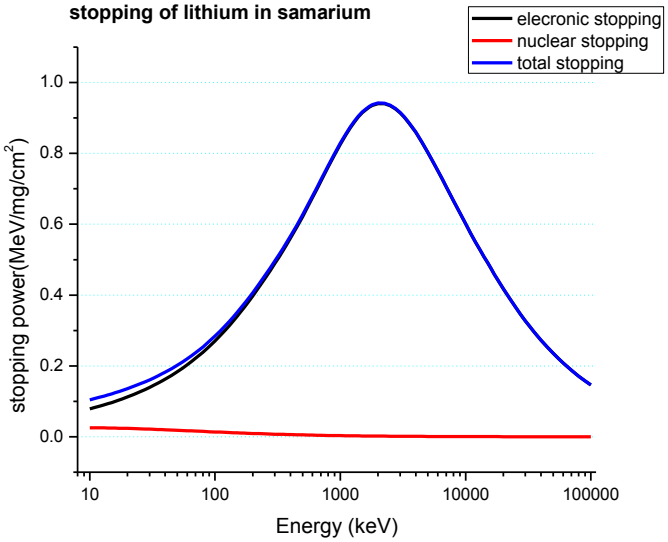
Fig4.2: Variation of stopping in Hydrogen with atomic number of target at different energies

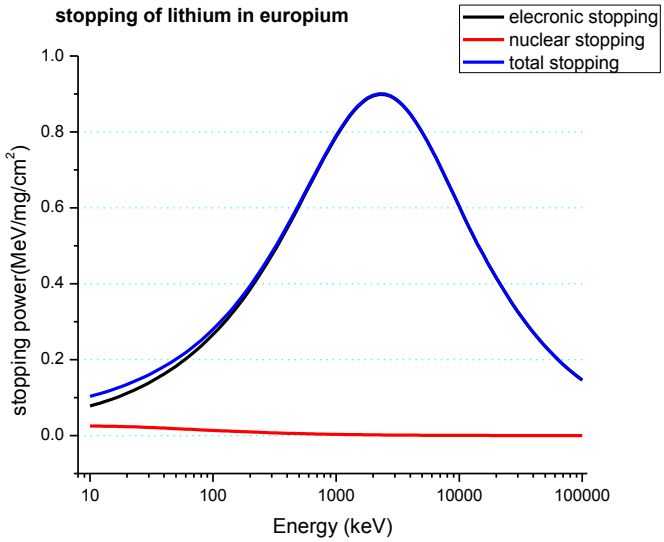
Stopping of lithium in lanthanide elements

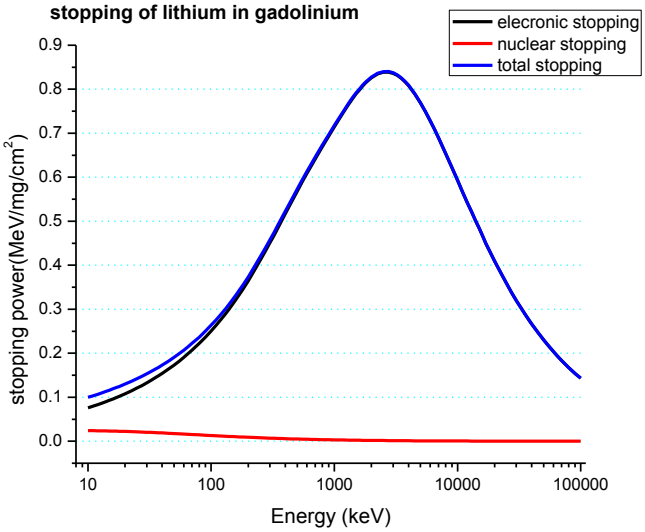
The following plots were obtained for stopping of lithium in lanthanides.

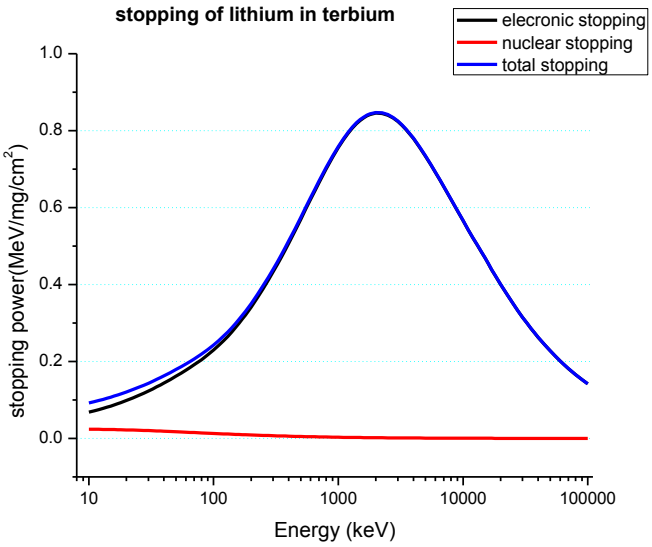


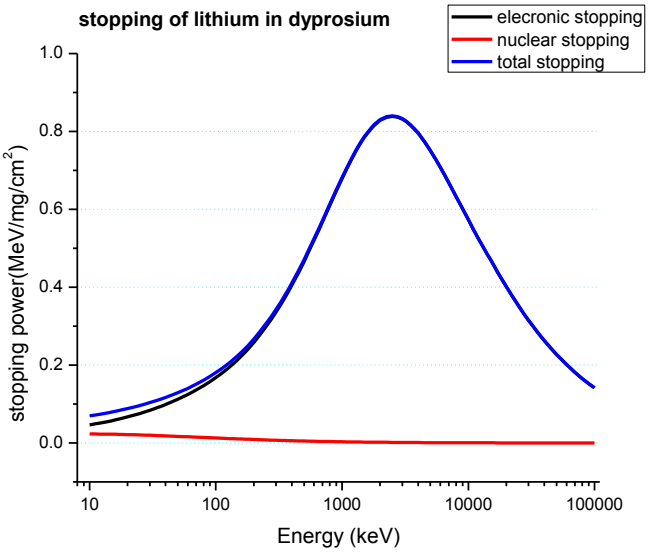

stopping of lithium in promethium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of lithium in samarium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of lithium in europium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of lithium in gadolinium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of lithium in terbium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of lithium in dyprosium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)

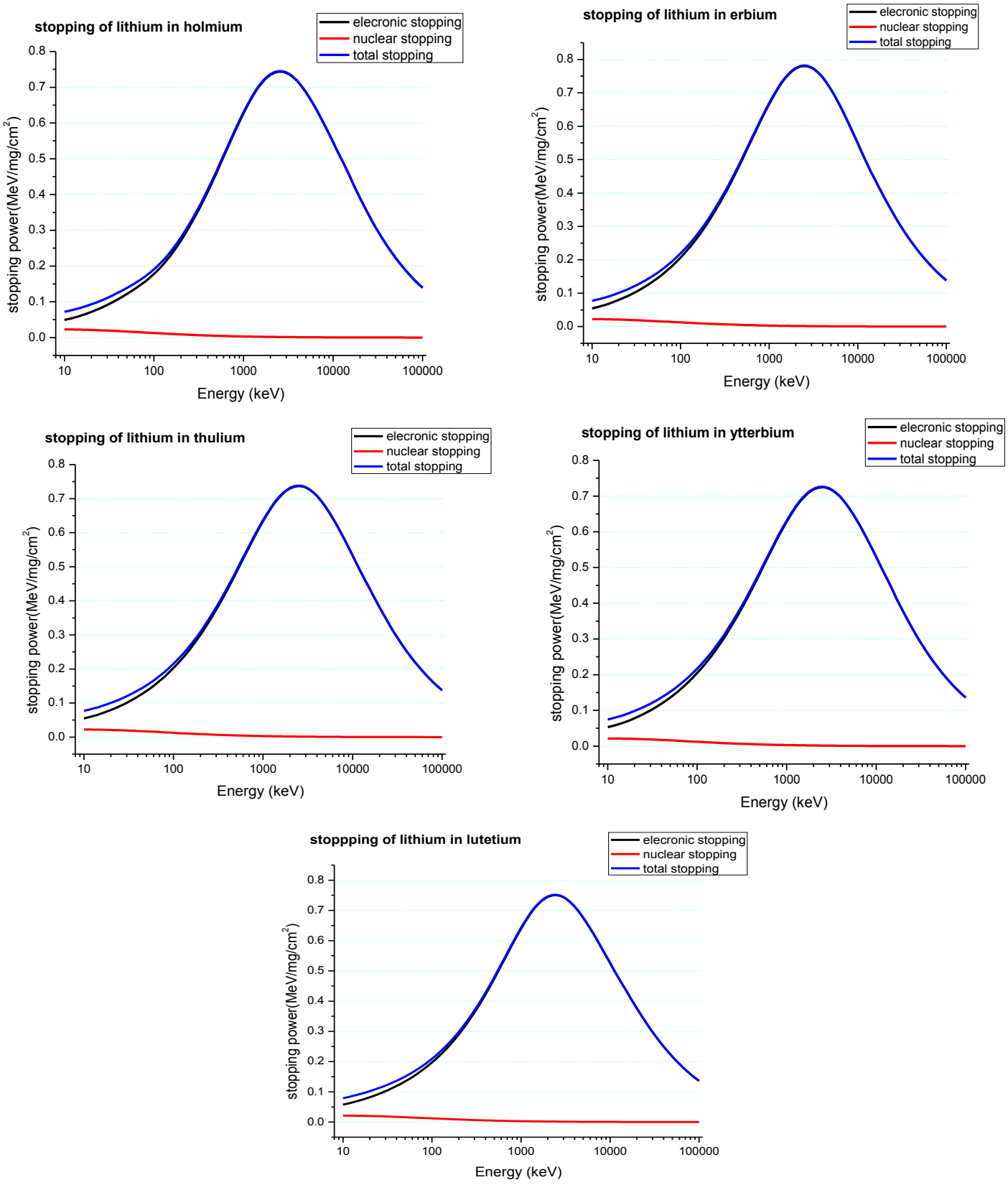


Fig4.3: Stopping of lithium in lanthanides

Electronic stopping follows the curve for total stopping except in low energies around 10keV to 100keV where there is a slight difference between electronic and total stopping. The stopping gradually increase till the peak is reached and then it decreases gradually. The peak lies between 1Mev to 10MeV. Nuclear stopping is always lower than the electronic stopping. The height of the peak decreases with increase in target atomic number indicating a decrease in stopping power.

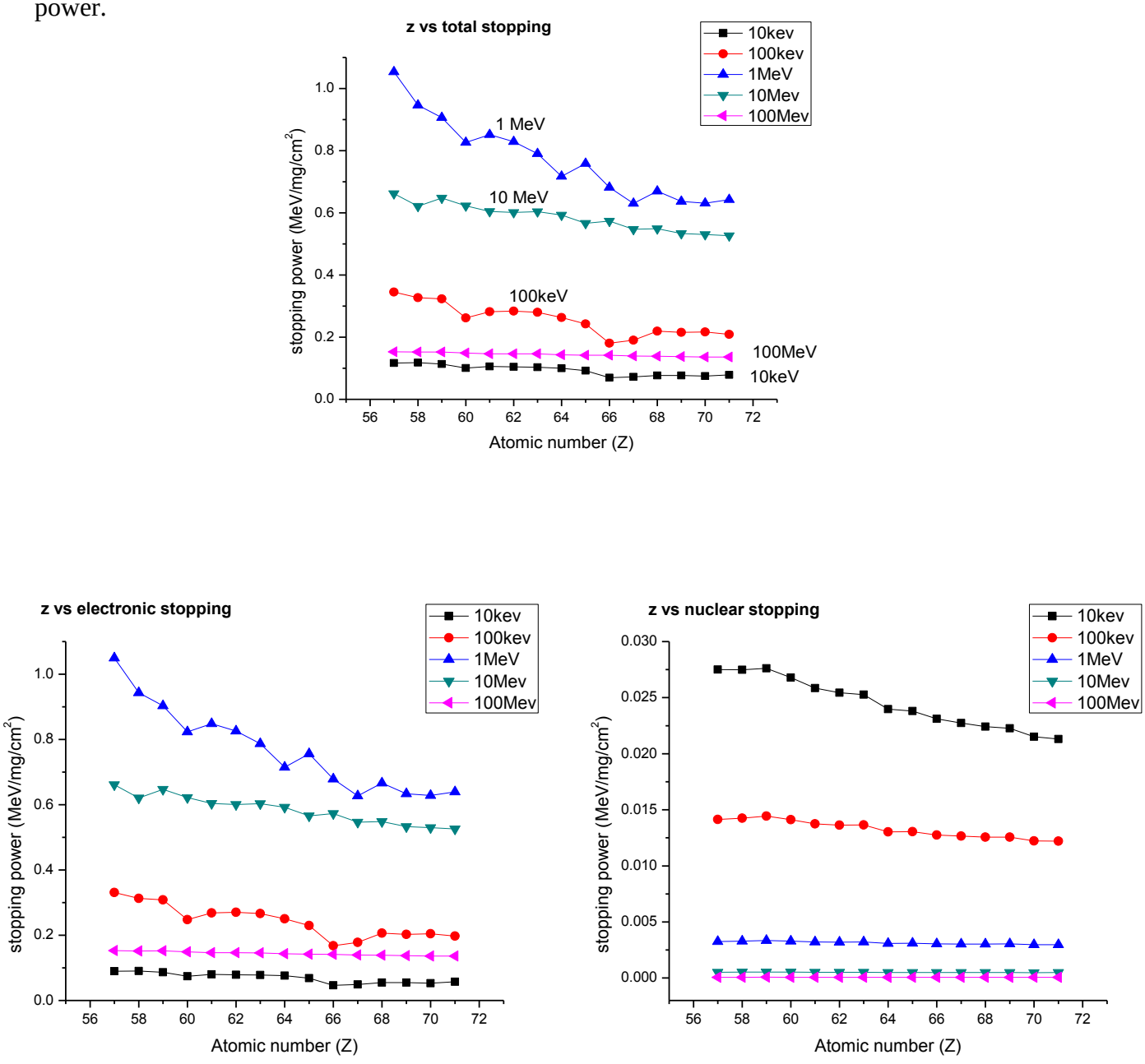
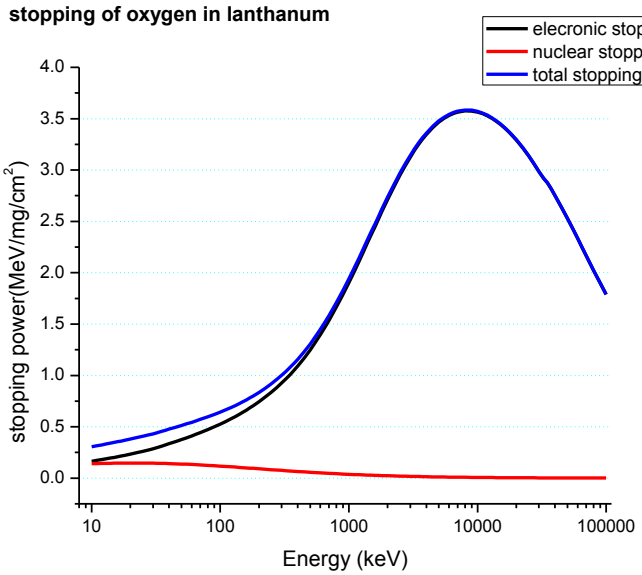


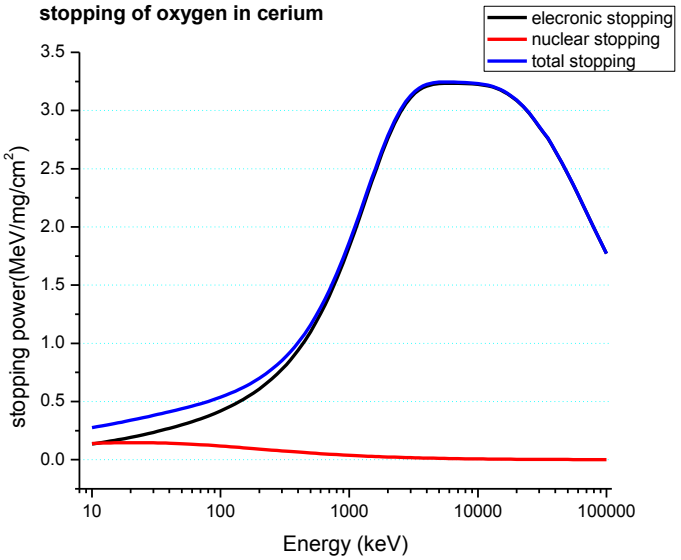
Fig4.4: variation of stopping power of lithium with atomic number of target

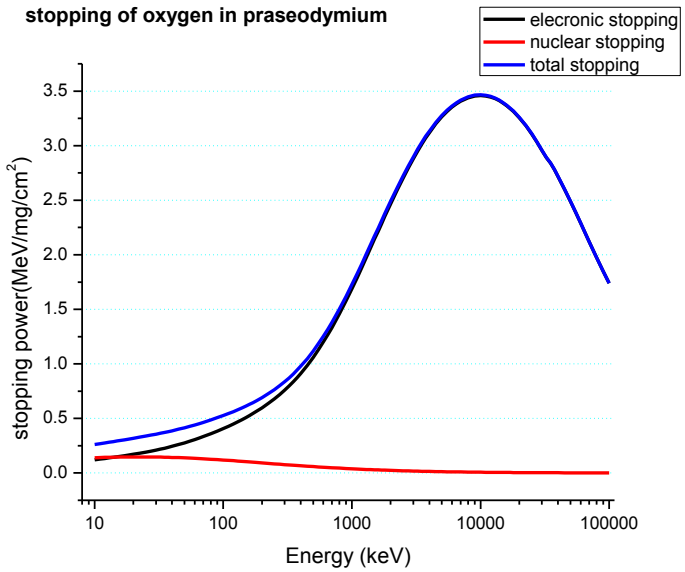
From the above plots we can see that all the stopping powers follow a decreasing trend with increase in atomic number of the target.

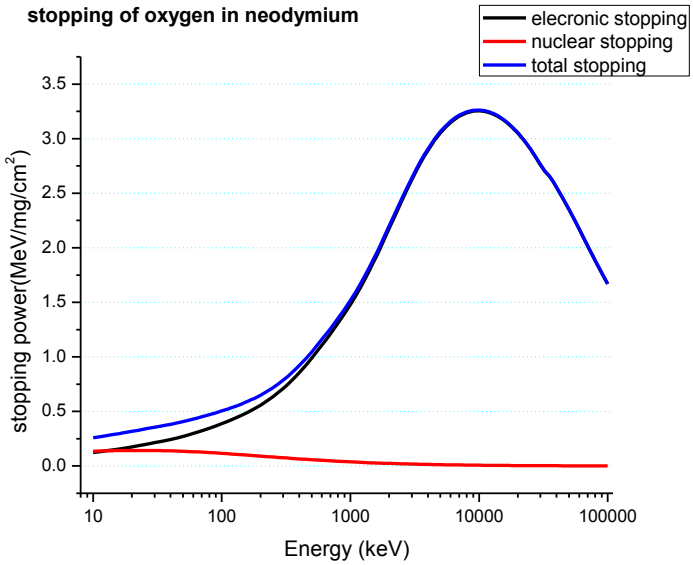
Stopping of oxygen in lanthanide elements

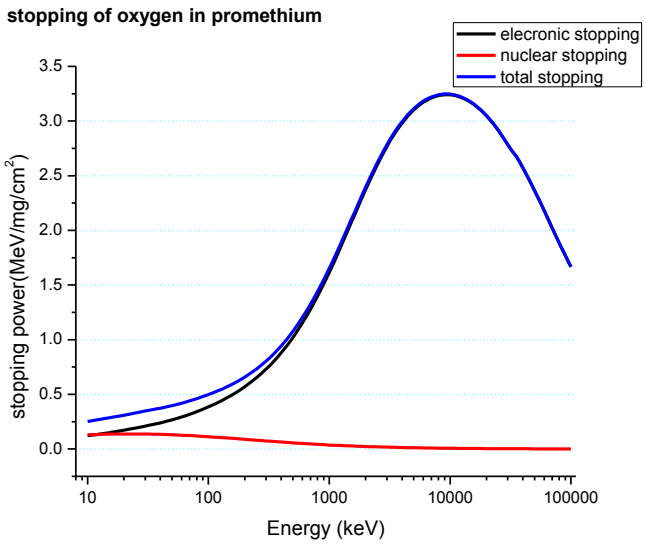
The following plots are obtained for stopping of oxygen in lanthanide elements.

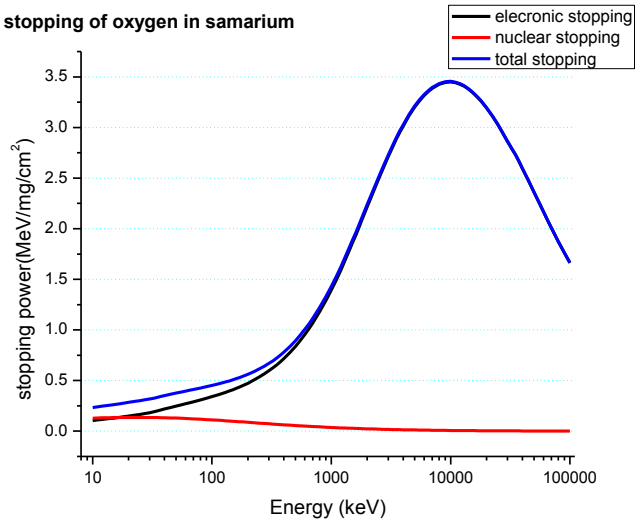


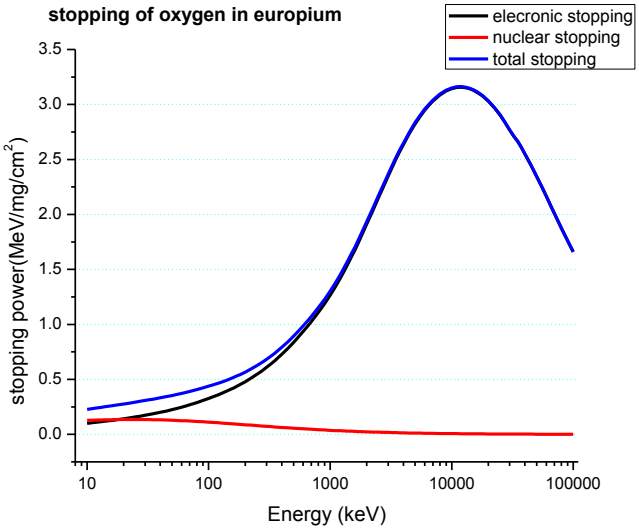


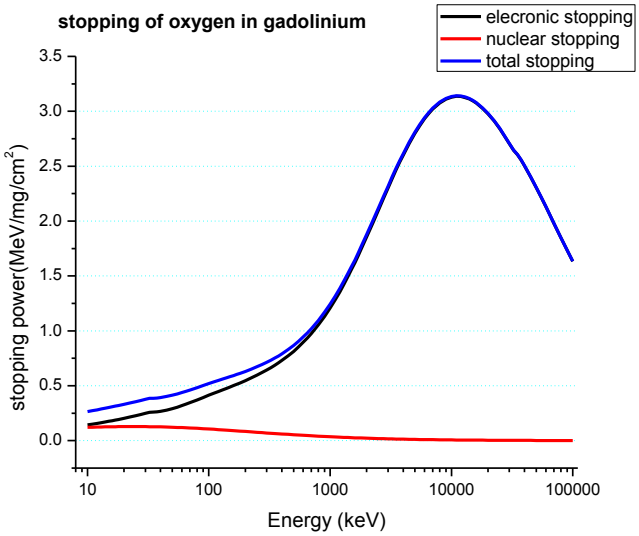


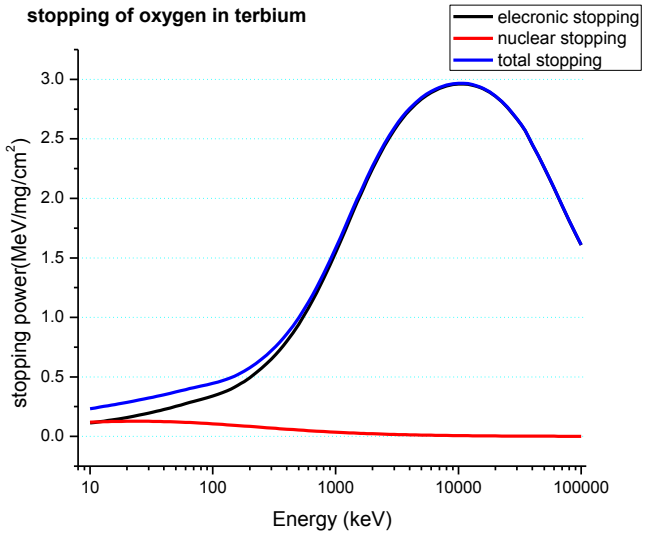


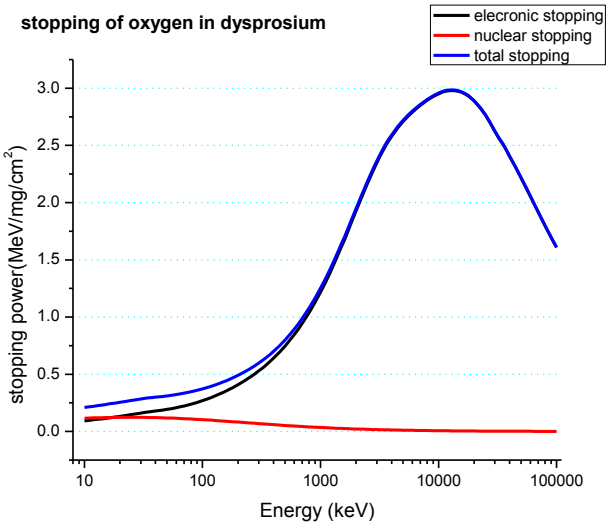

stopping of oxygen in promethium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)

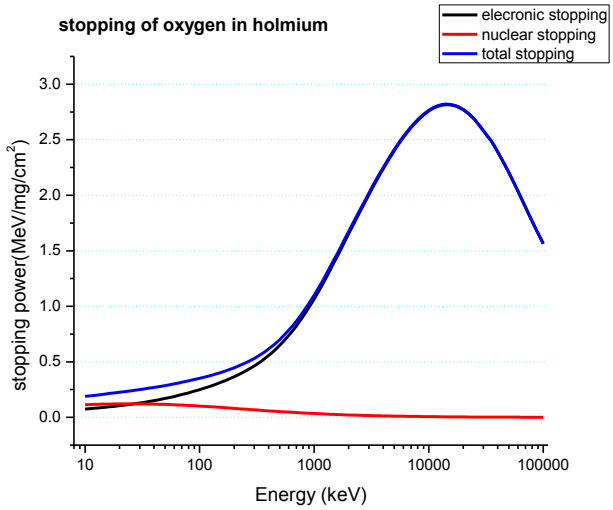

stopping of oxygen in samarium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)

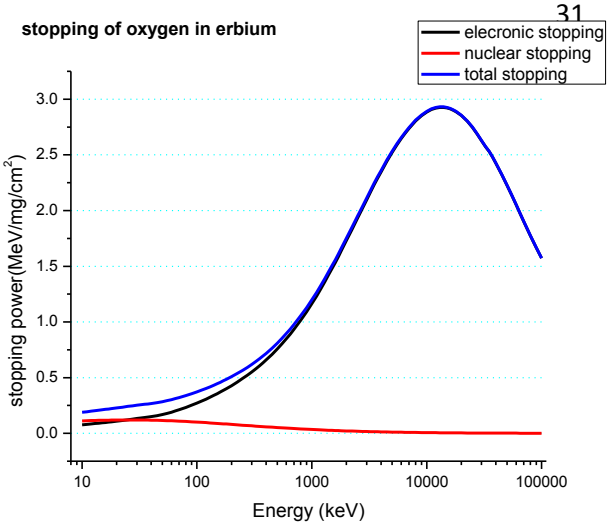

stopping of oxygen in europium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)

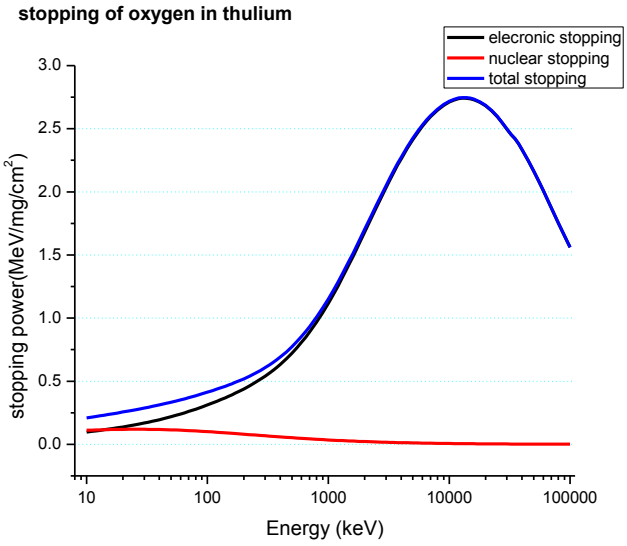

stopping of oxygen in gadolinium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)

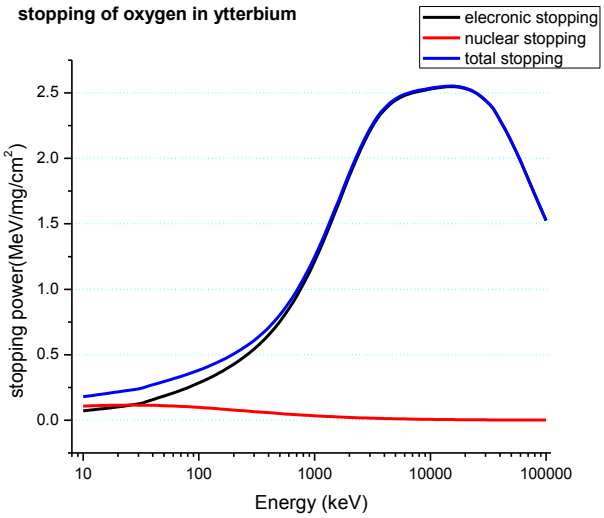

stopping of oxygen in terbium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of oxygen in dysprosium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)









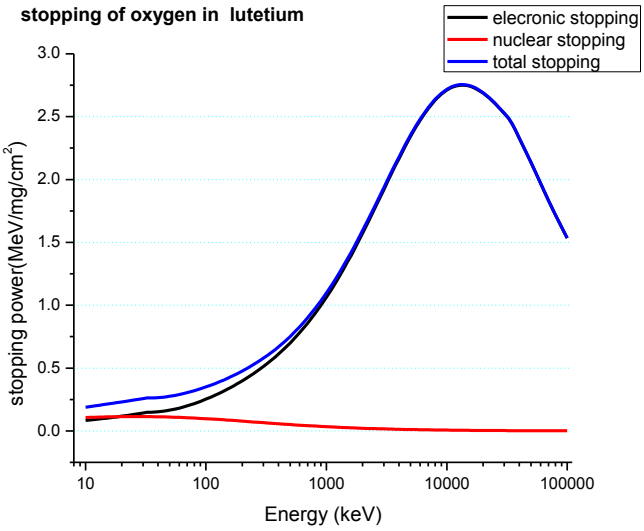


Fig4.5: Stopping of oxygen in lanthanide elements

For lower energies there is a distinct difference between the electronic and total stopping. For very low energy i.e. around 10keV the nuclear stopping is more than the electronic stopping. The nuclear stopping distinctively decreases with increase in energy of the ion. The stopping is very low at low energies. The electronic stopping gradually increases till it peaks around 10MeV and then it starts gradually decreasing. From the plots below it is evident that all stopping decreases with increase in atomic number of target.

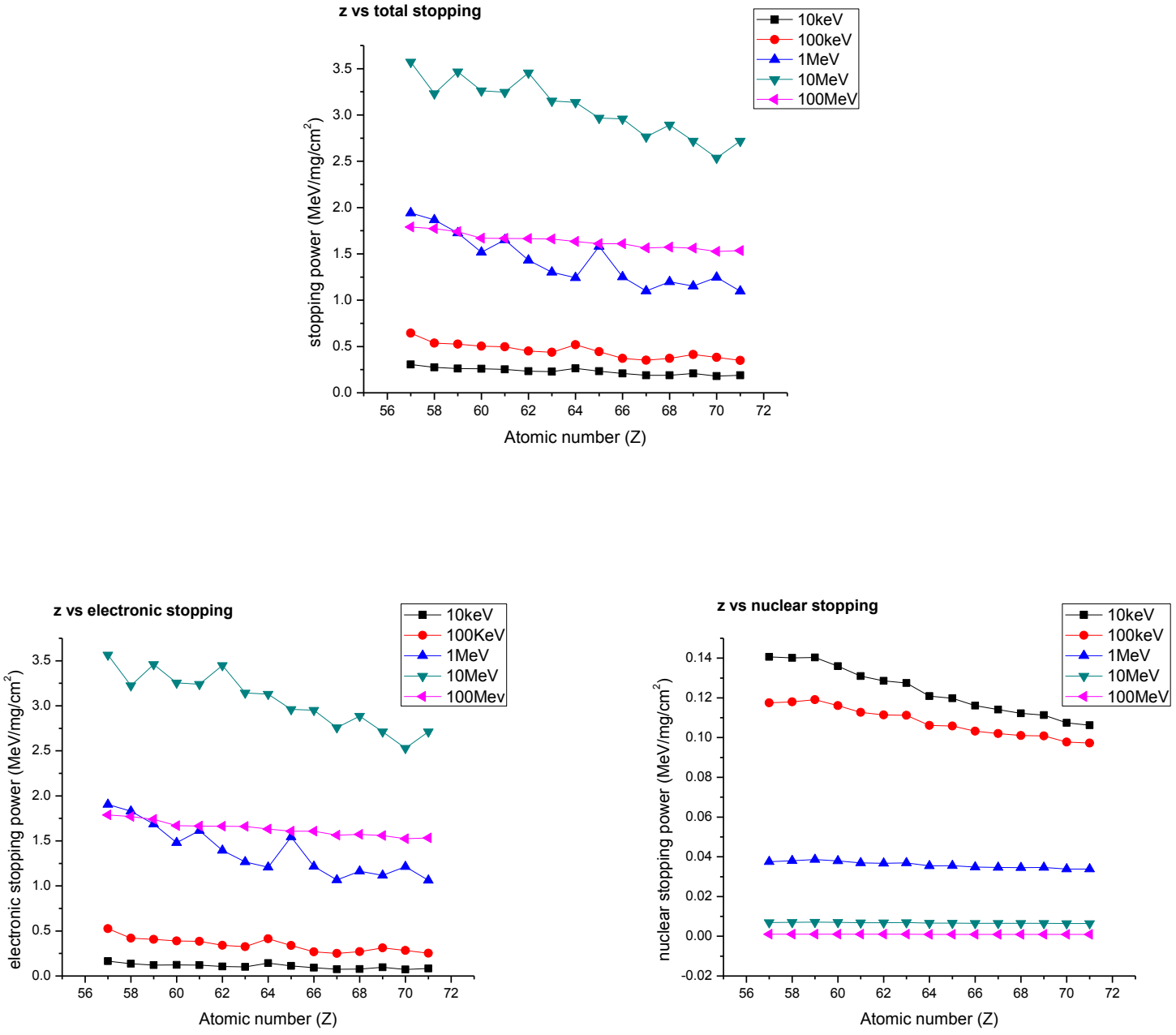
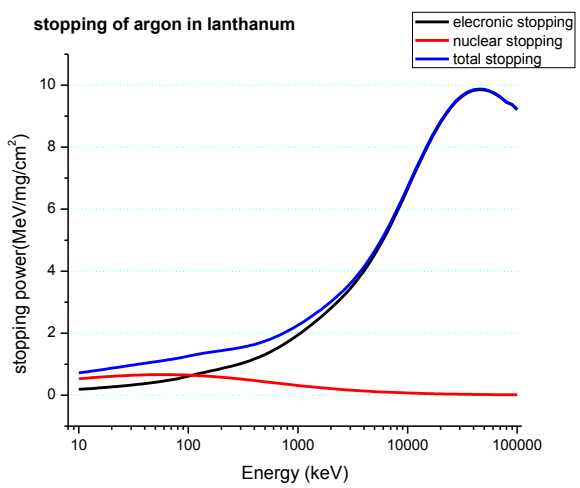
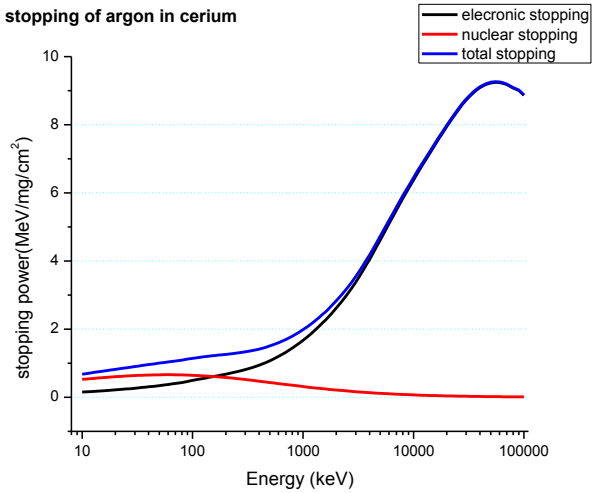


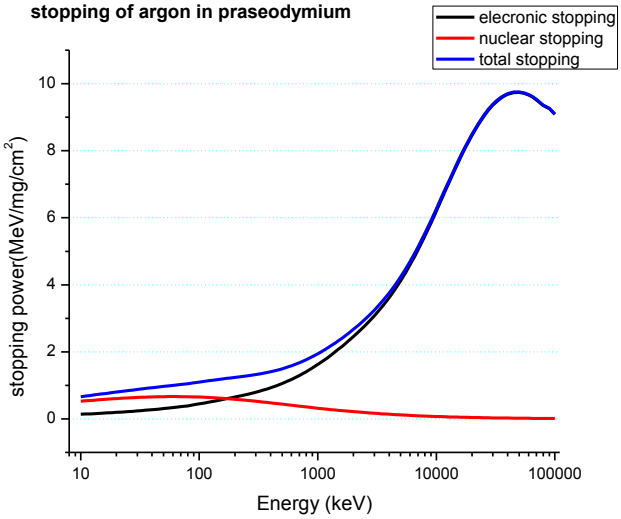
Fig4.6: variation of stopping of oxygen with atomic number of target

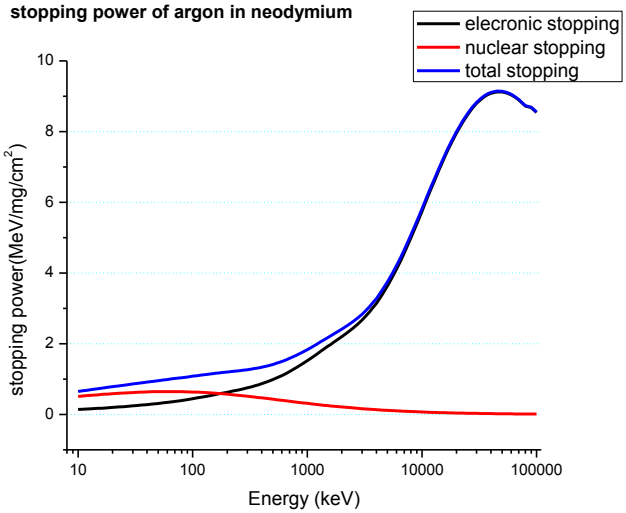
Stopping of Argon in lanthanide elements

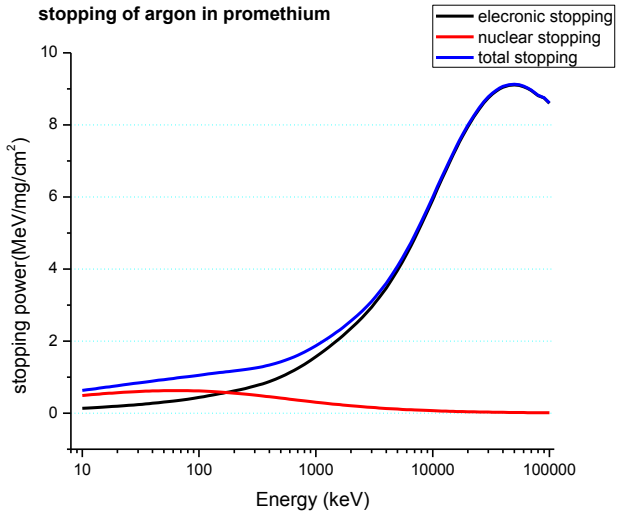
The following plots are obtained for stopping power of Argon in the lanthanides.

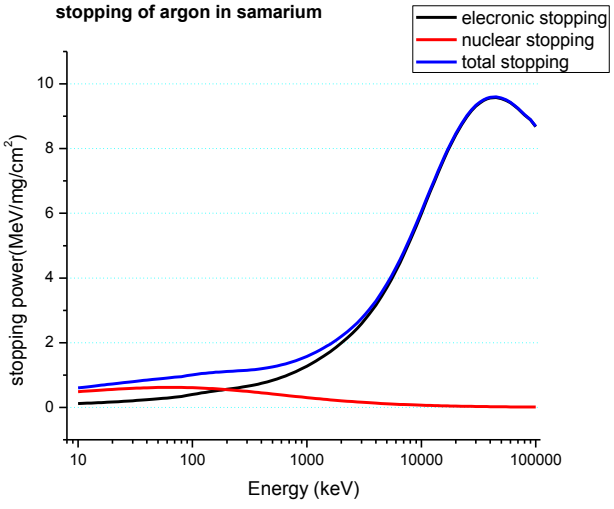


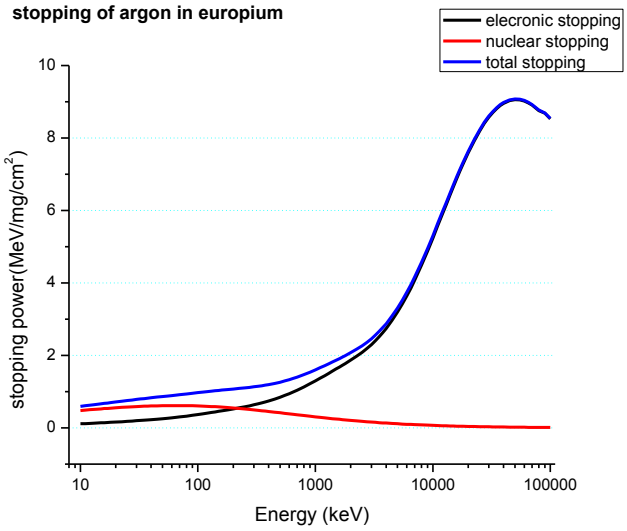


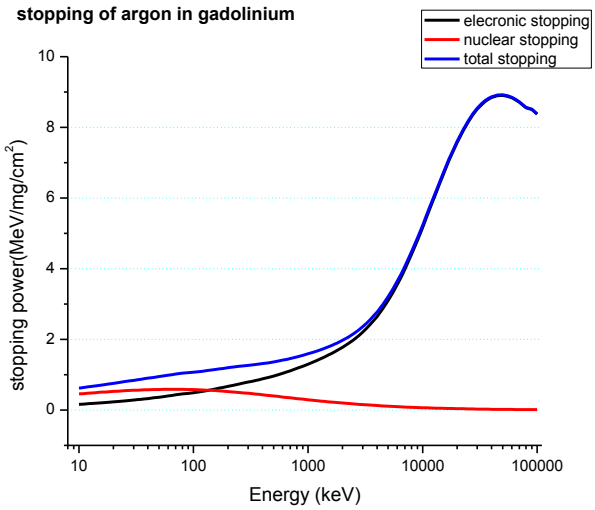


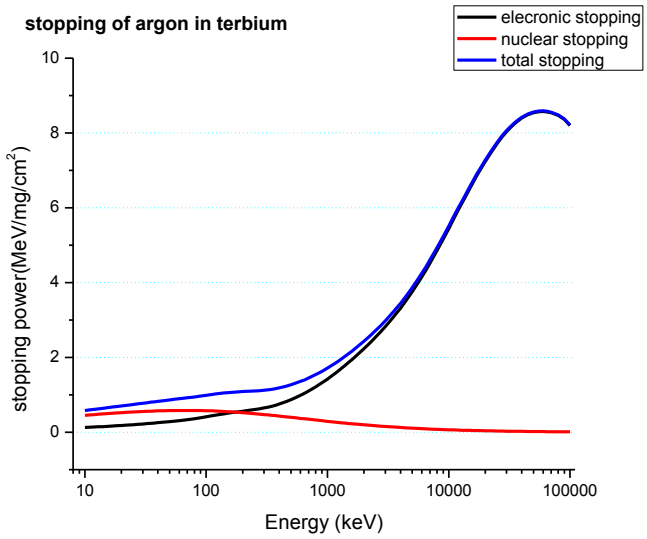


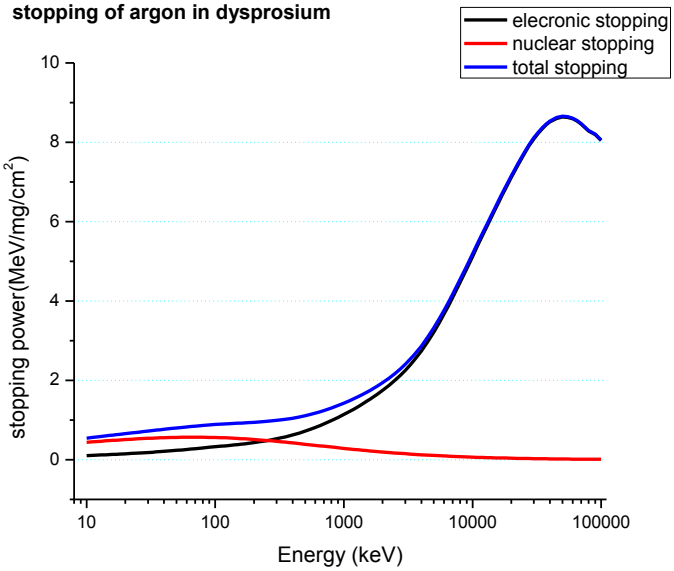


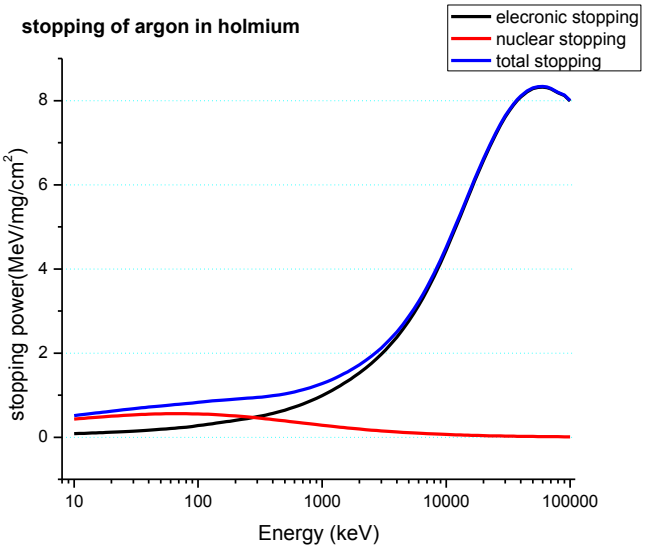


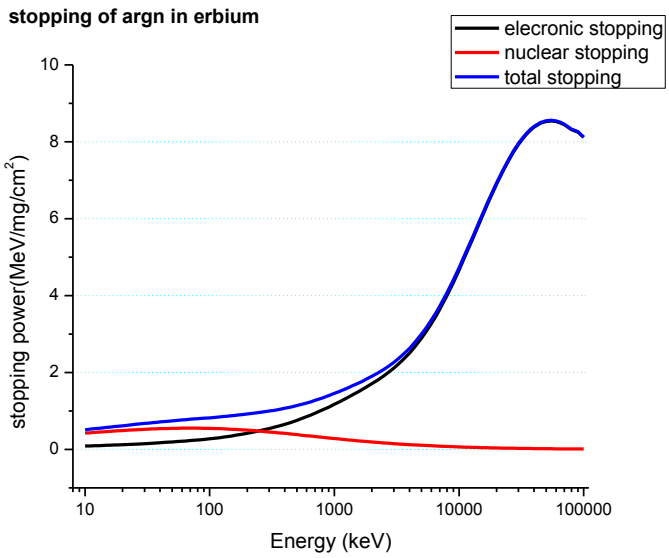

stopping of argon in europium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of argon in gadolinium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of argon in terbium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of argon in dysprosium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of argon in holmium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)


stopping of argn in erbium
elecronic stopping
nuclear stopping
total stopping
stopping power(MeV/mg/cm2)
Energy (keV)

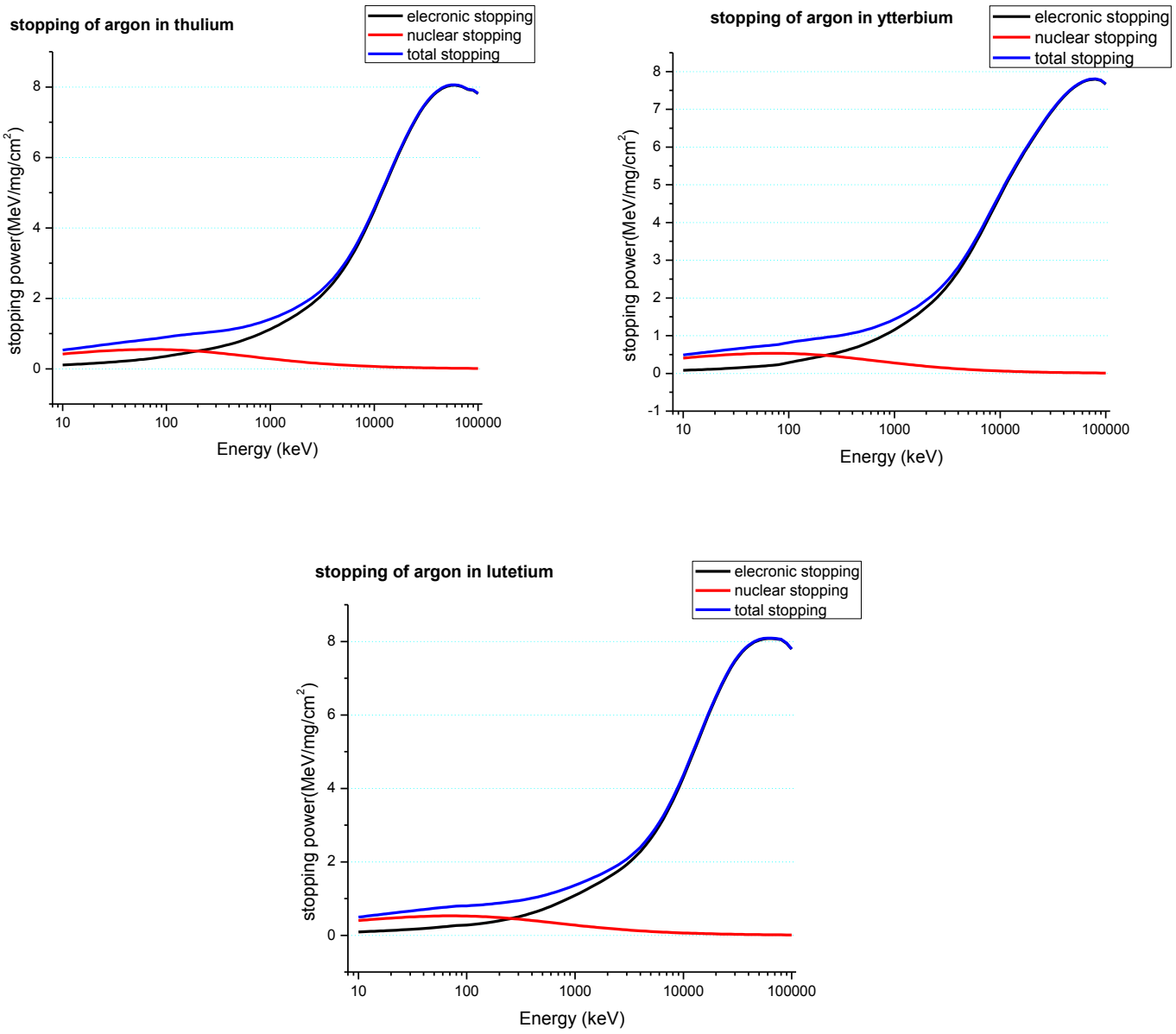


Fig4.7: stopping of argon in lanthanide elements

In lower energies the nuclear stopping is more than electronic stopping hence it contributes more to the total stopping in lower energy. At some point between 100keV and 1MeV the electronic stopping becomes more and then it follows the curve of total stopping. The stopping power achieves a peak at around 30MeV. The value of the stopping at the peak decreases with increasing atomic number of the target, therefore it indicates the stopping follows a decreasing trend. The nuclear stopping decreases after 100keV and hence its contribution to the total stopping is negligible in higher energies of the incident ion. The graphs below plot the variation of the stopping with atomic number of the target. It is evident that all the stopping follows a decreasing trend with the increase in target atomic number.

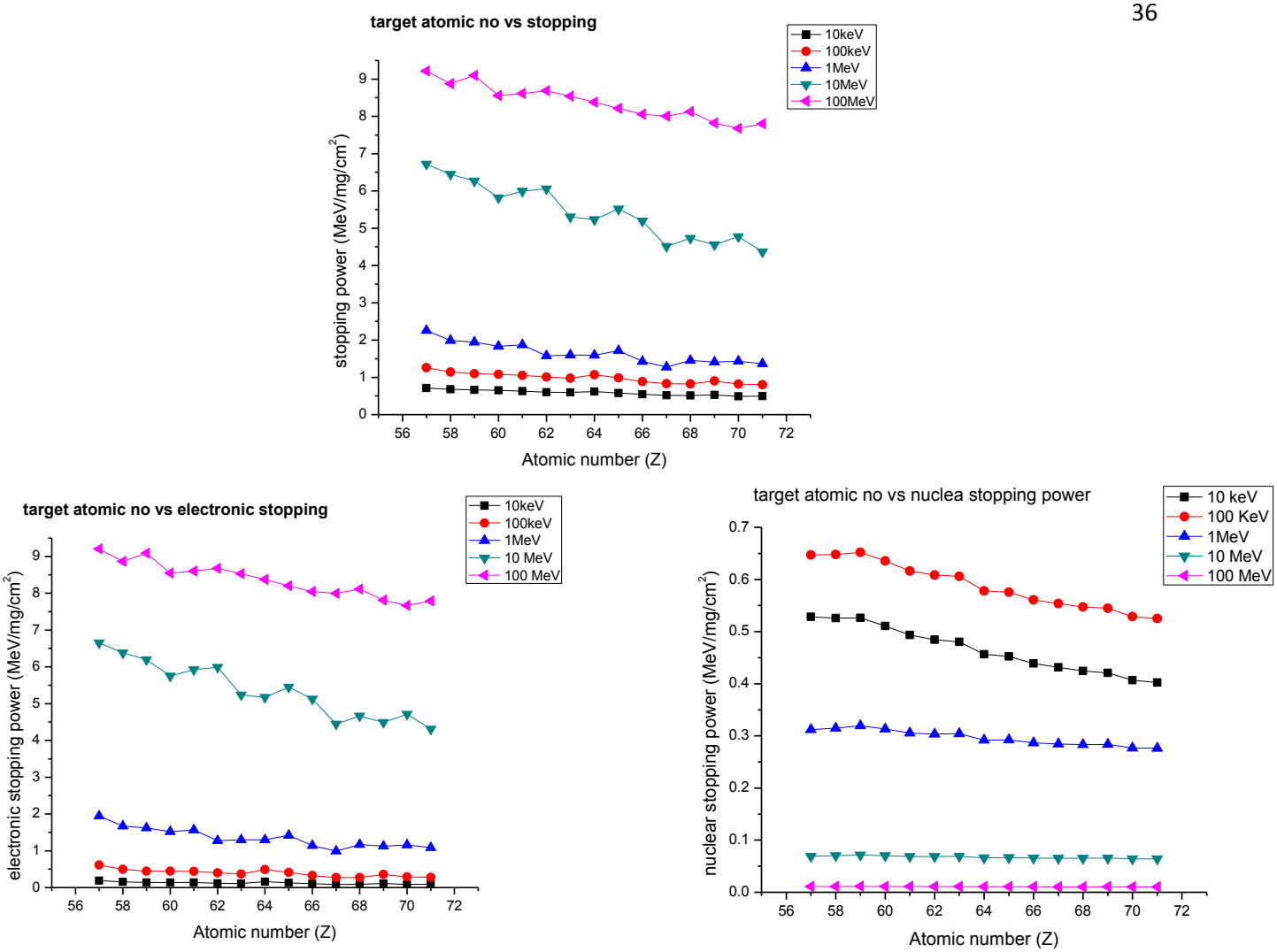
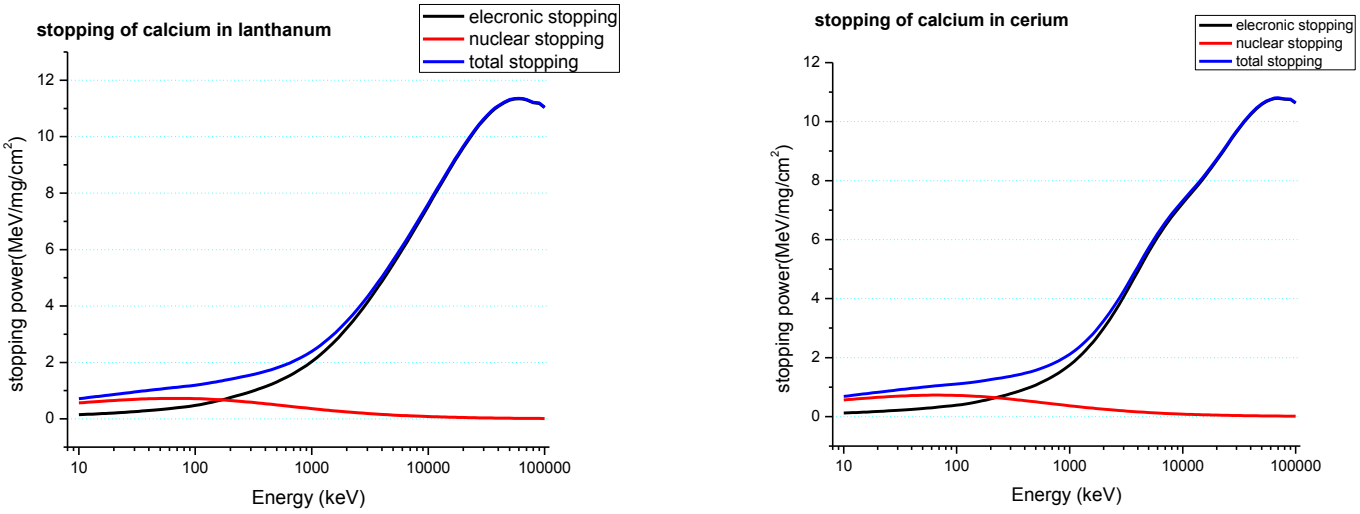


Fig4.8: variation of stopping of argon with atomic number of target

Stopping of calcium ion in lanthanide elements

The following plots are obtained for stopping power of Calcium in the lanthanides.



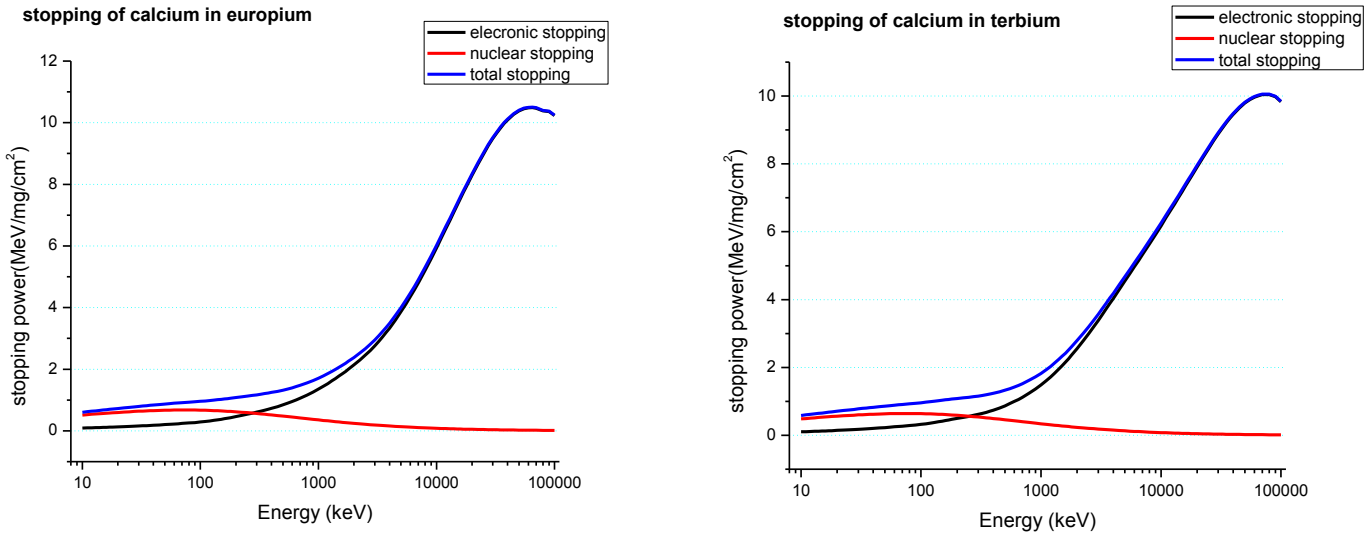
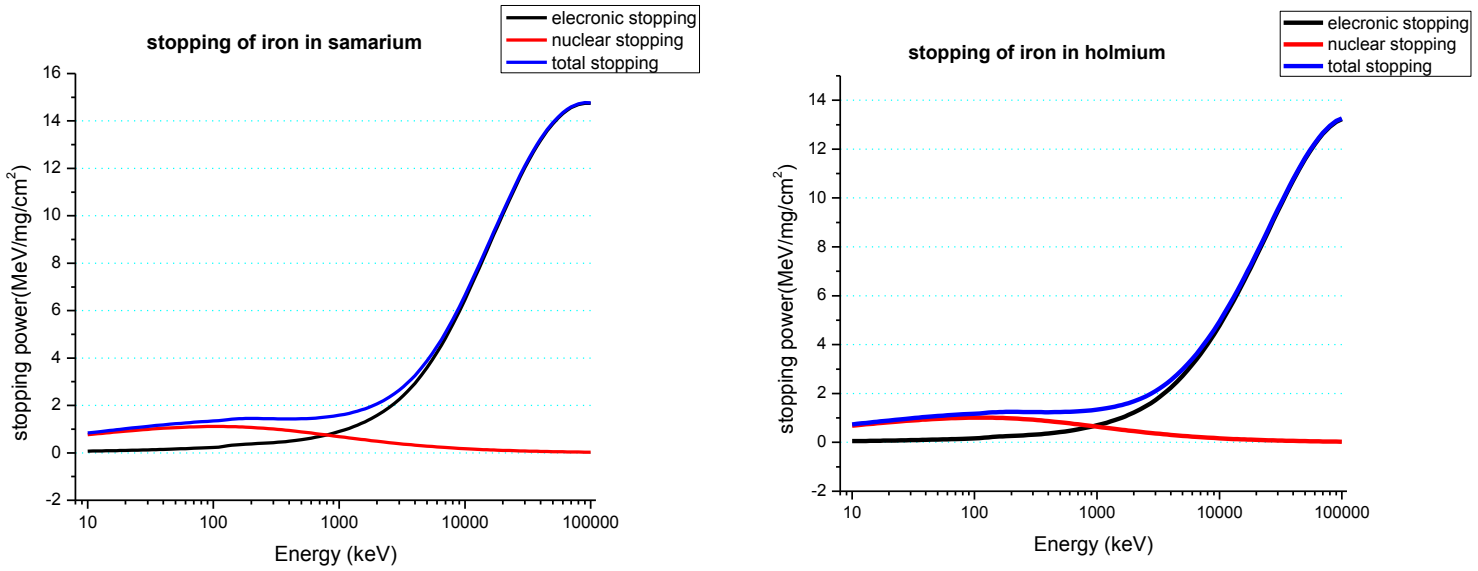


Fig4.9: stopping of calcium in some lanthanides

The stopping gradually increases upto approximately 40MeV and then decreases slowly after. The nuclear stopping is more than electronic stopping in lower energies. It increases upto 100keV and then decreases after. Up until a point between 100keV to 1MeV nuclear stopping contributes to total stopping more than electronic stopping. As in the previous ions the stopping of Calcium also decreases along with increase in atomic number as is evident from the lowering of the value of the peak.

Stopping of iron in lanthanide elements

The following are a few plots depicting the stopping of iron in a few lanthanide elements.



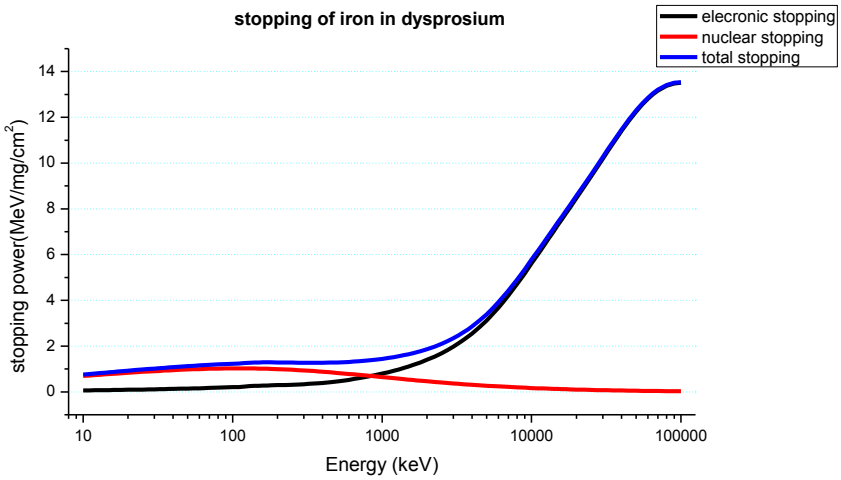
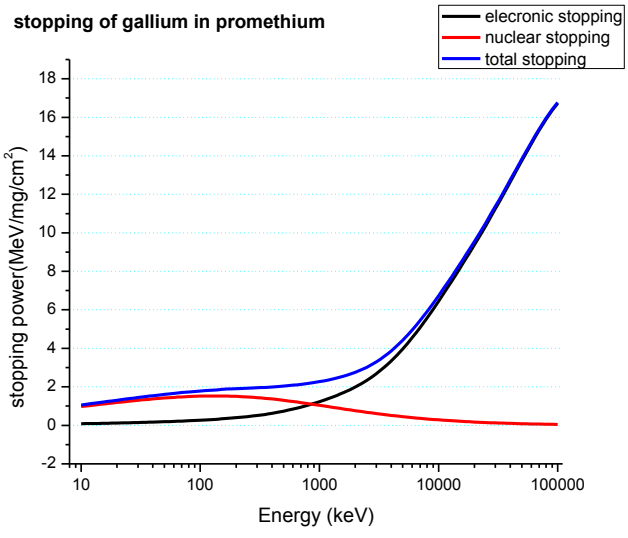


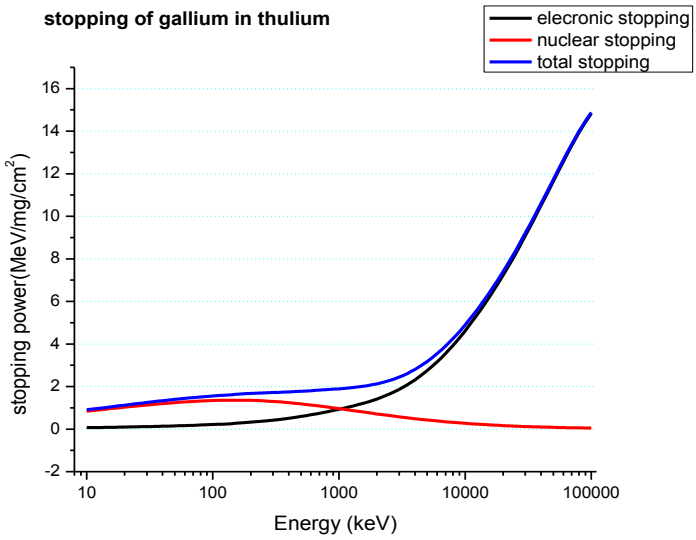
Fig4.10: stopping of iron in a few lanthanide elements

At around 1MeV the nuclear stopping becomes less than electronic stopping. The electronic stopping is low for lower energies but increases gradually to follow the curve of total stopping. The increase in electronic stopping is gradual for lower energies but increases rapidly once the energy of the ion crosses around 10MeV. As in the case of previous ions the stopping decreases with increase in atomic number of target.

Stopping of gallium in lanthanide elements

The following are a few plots depicting the stopping of gallium in a few lanthanide elements.





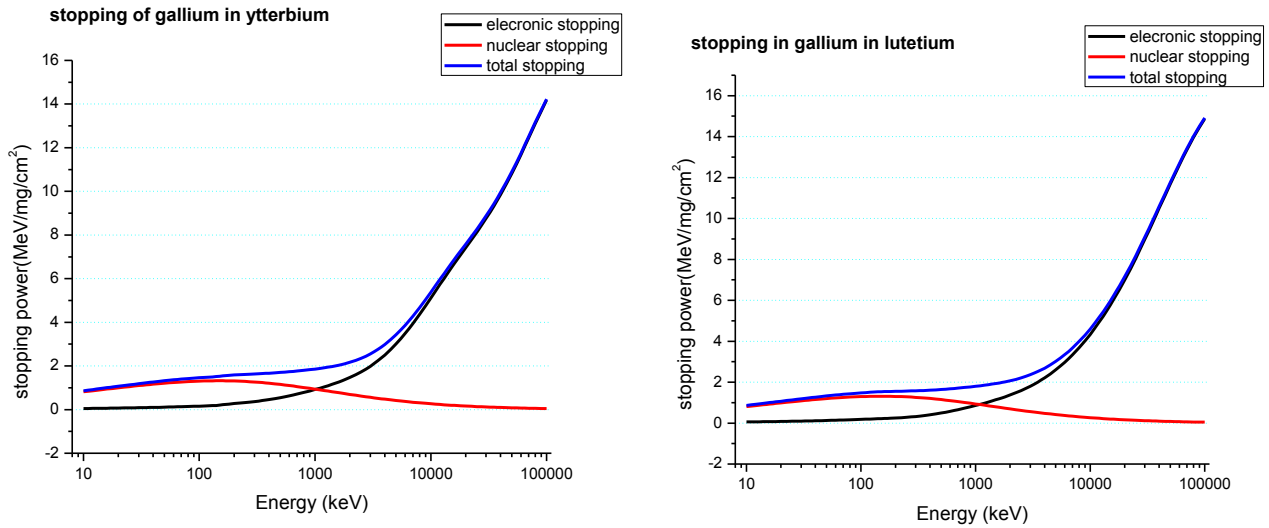


Fig 4.11: stopping of gallium in few lanthanide elements

Electronic and total stopping follow the same path except for energies lower than 10MeV, where the electronic power is significantly lower. The stopping increases gradually till around 20MeV, and then there is a rapid increase after that. The peak lies beyond 100MeV. Nuclear stopping increases till around 100keV and then it gradually decreases as the energy of the ion increases.

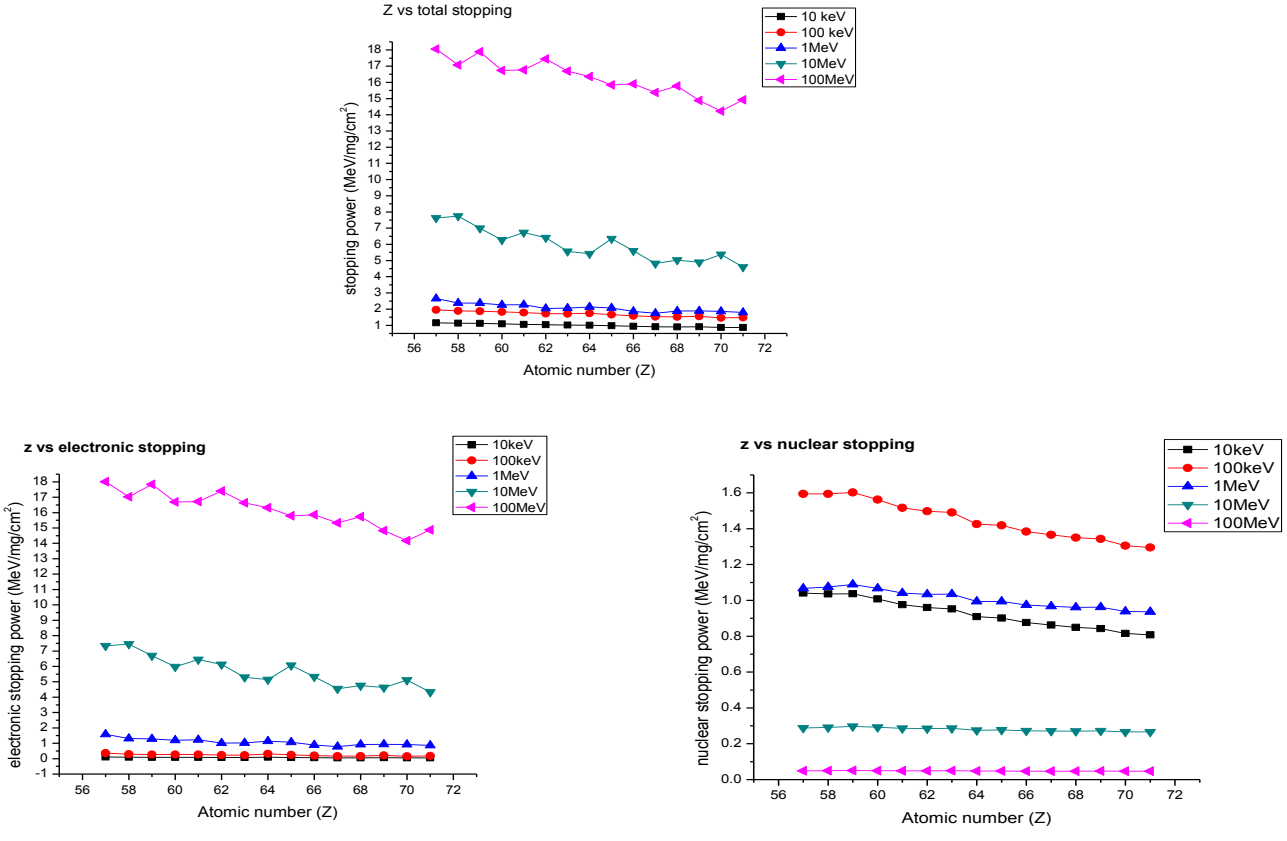


Fig4.12: variation of stopping of gallium with atomic number of target.

All the stopping have a decreasing trend with the increase in atomic number as seen from the plots above. As can be seen from the third plot, the nuclear stopping increases till 100keV, and then decreases for higher energies.

Stopping of Arsenic in lanthanide elements

The following are a few plots depicting the stopping of arsenic in a few lanthanide elements.

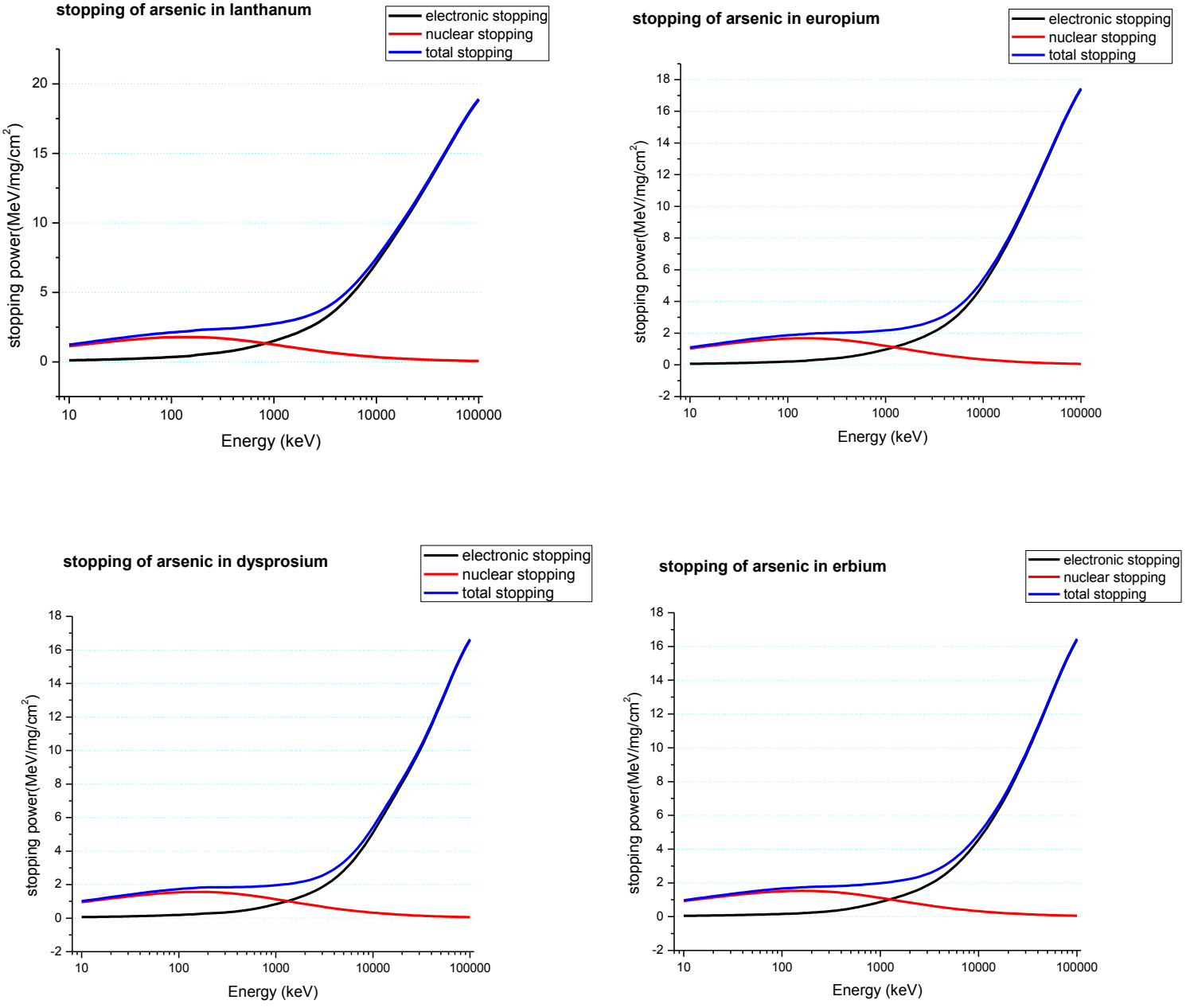


Fig4.13: stopping of arsenic in a few lanthanide elements

The electronic stopping follows the curve of total stopping for higher energies but there is a distinct difference between the two for energies lower than 10MeV. Electronic stopping increases in a staggered manner till around 10MeV and then it rapidly increases. The total stopping dips slightly near 1MeVand then increases rapidly. The peak lies beyond 100MeV. The nuclear stopping is highest around 100keVand decreases as the energy of the ion decreases.

Stopping of gold in lanthanide elements.

The following are a few plots depicting the stopping of gold in a few lanthanide elements.

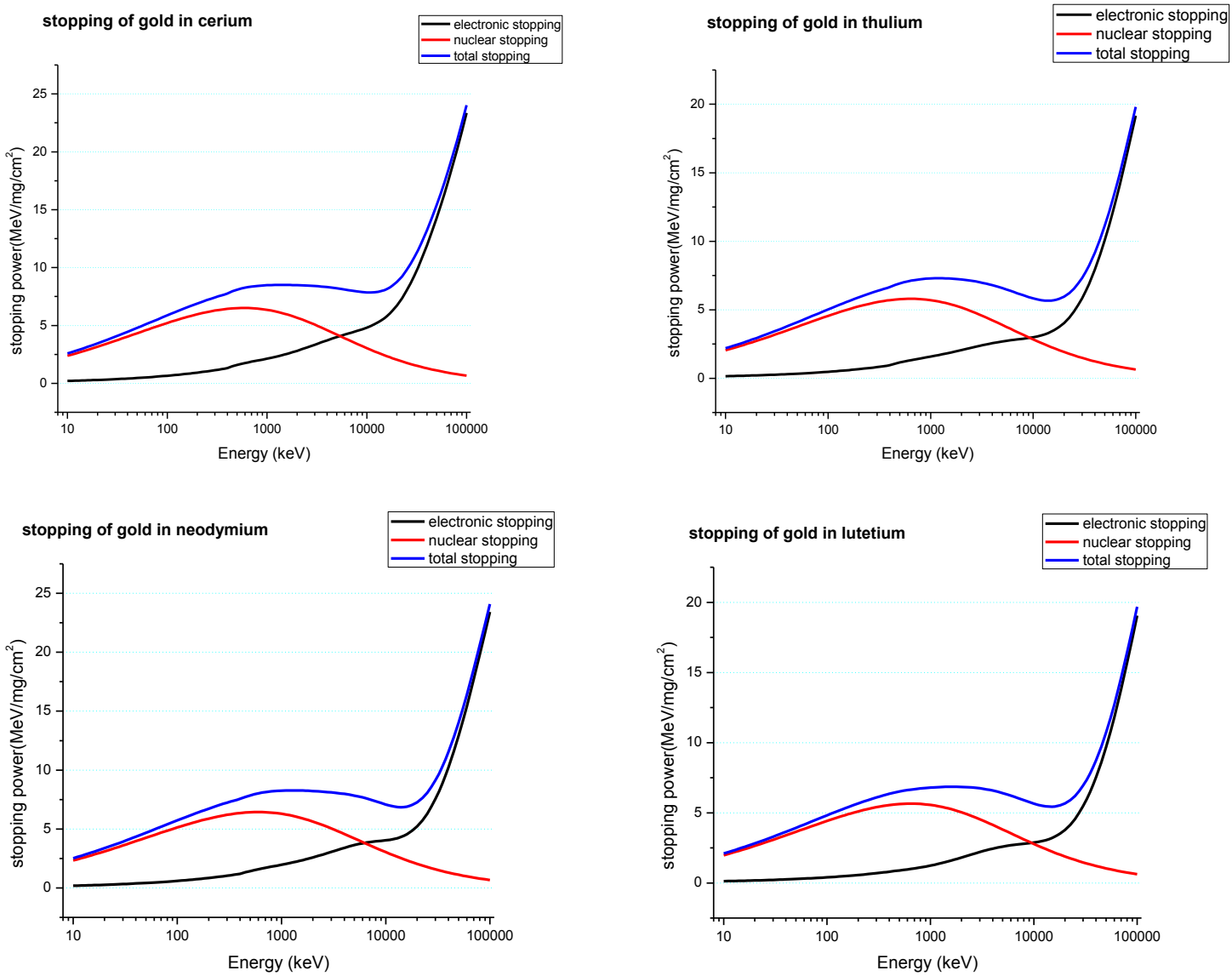
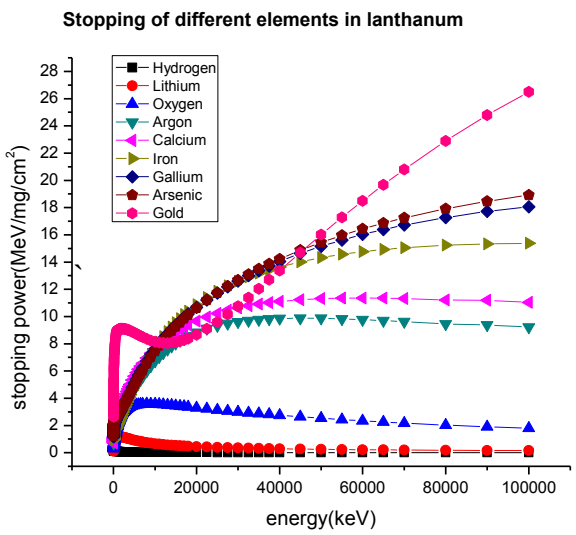
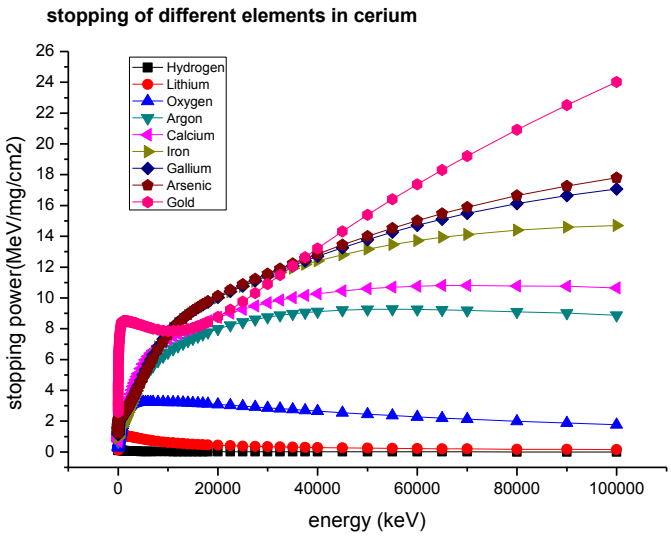


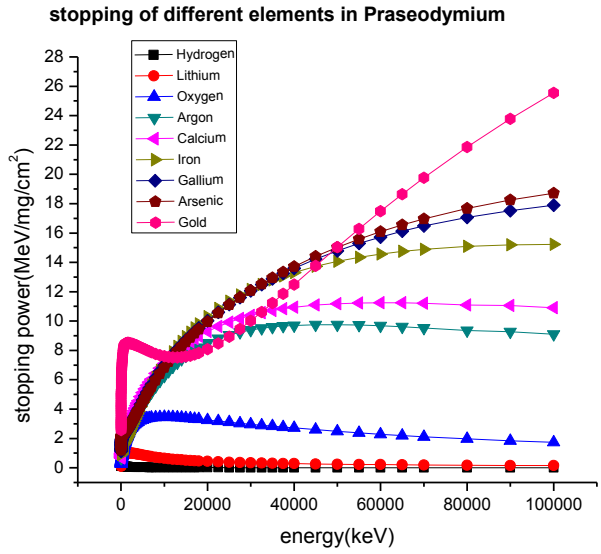
Fig4.14: stopping of gold in few lanthanide elements

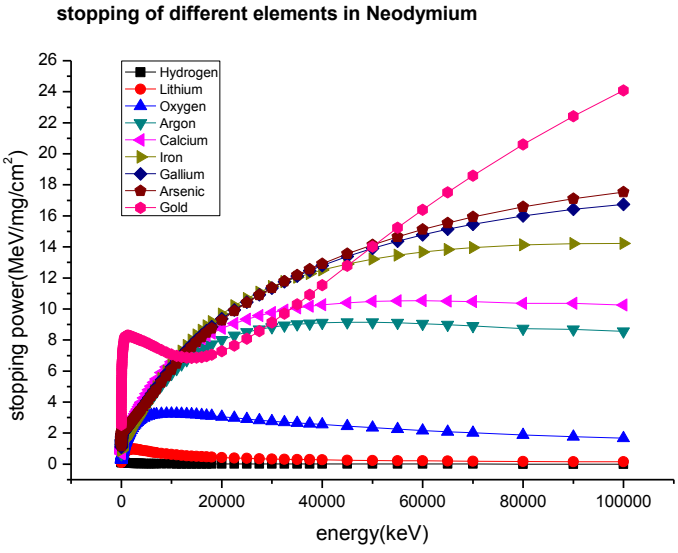
The nuclear stopping becomes more than electronic stopping after 10MeV. Electronic stopping increases gradually till approximately 10MeV then there is a rapid increase. Total stopping gradually increases till 1MeV then decreases to form a dip around 10MeV and then rapidly increases after. Nuclear stopping increases gradually till 1MeV and then gradually decreases after. Nuclear stopping follows the total stopping curve for lower energies (~100keV) of the incident ion whereas the electronic stopping follws the total energy curve for higher energies (>>10MeV).

In the plots given below the stopping from the different ions are grouped together in each of the lanthanide elements. It gives clear understanding of how the stopping varies for the different projectiles.

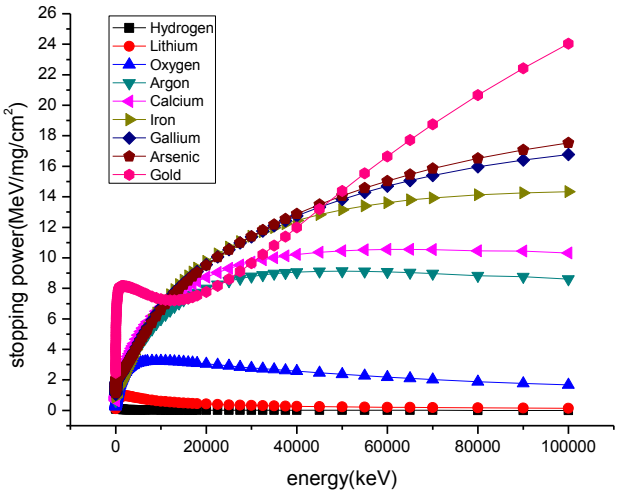




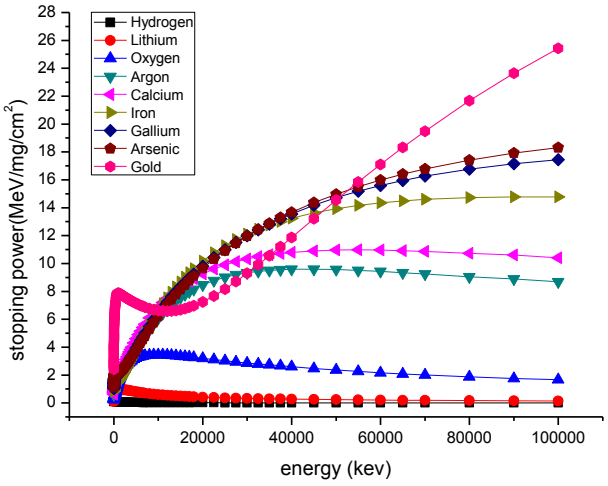




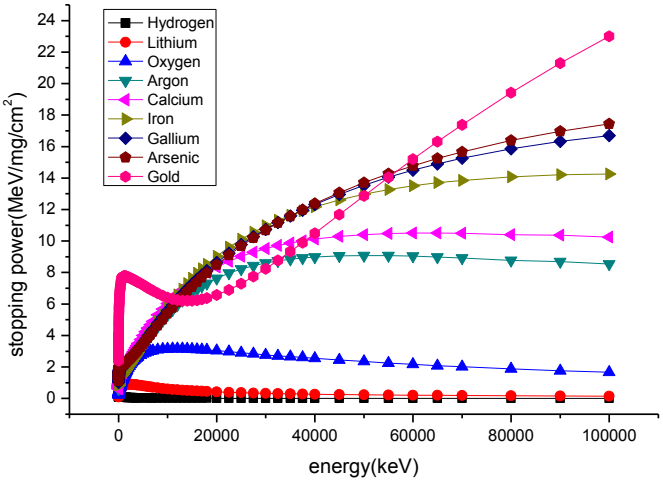
stopping of different elements in promethium



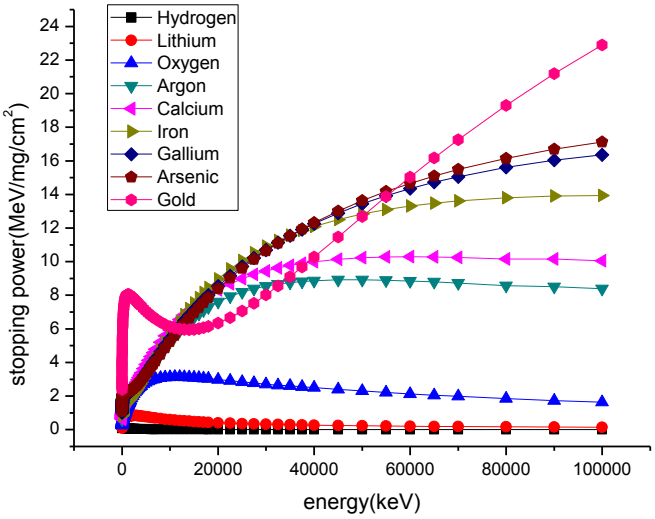
stopping of different elements in samarium



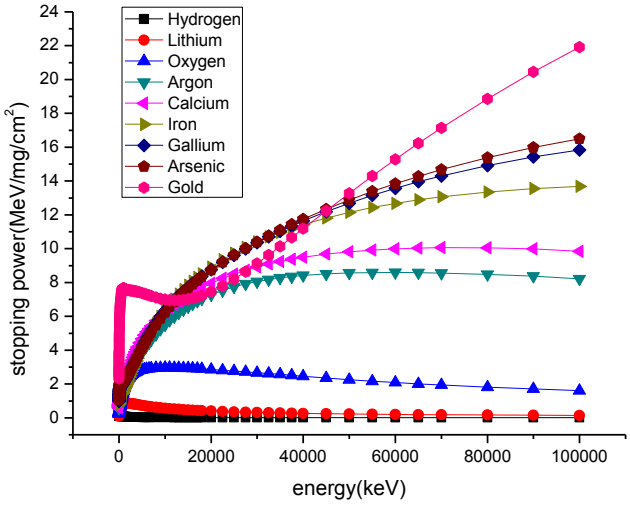
stopping of different elements in europium



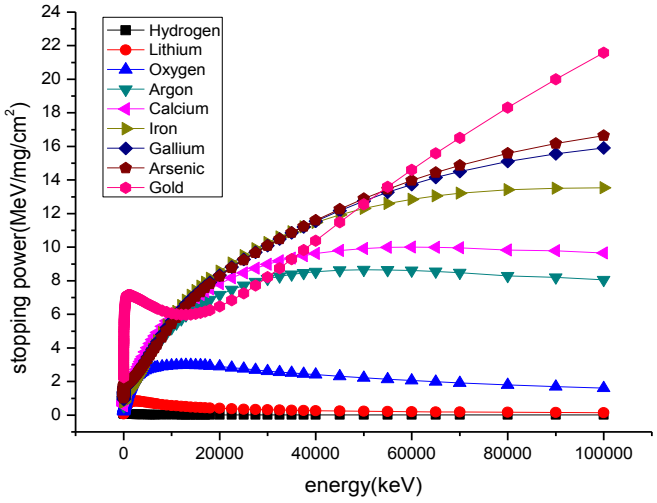
stopping of elements in gadolinium



stopping of elements in terbium



stopping of elements in dysprosium



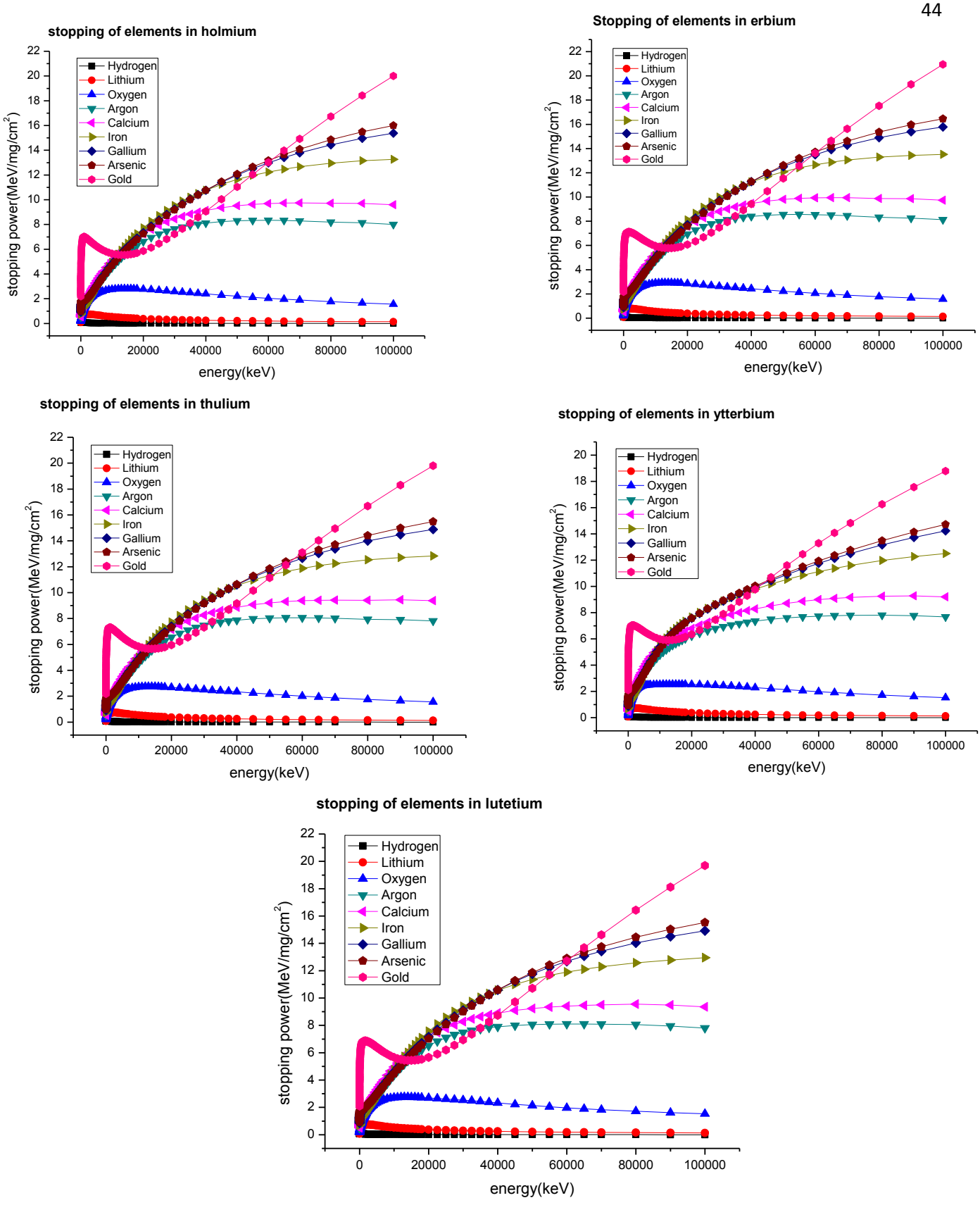
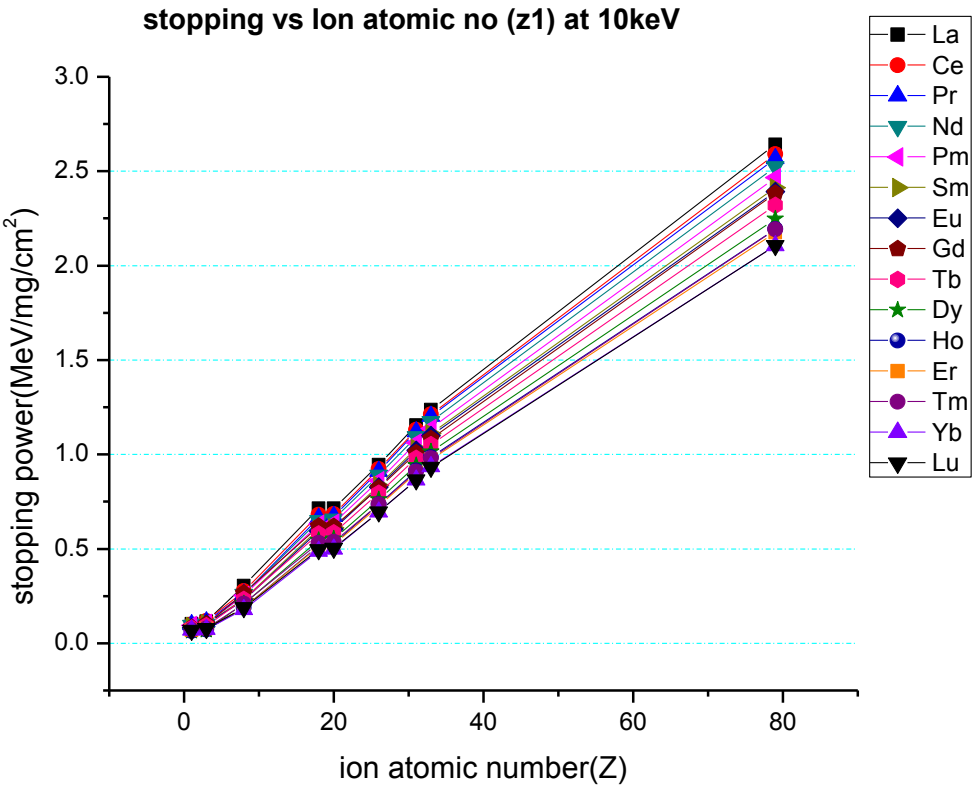
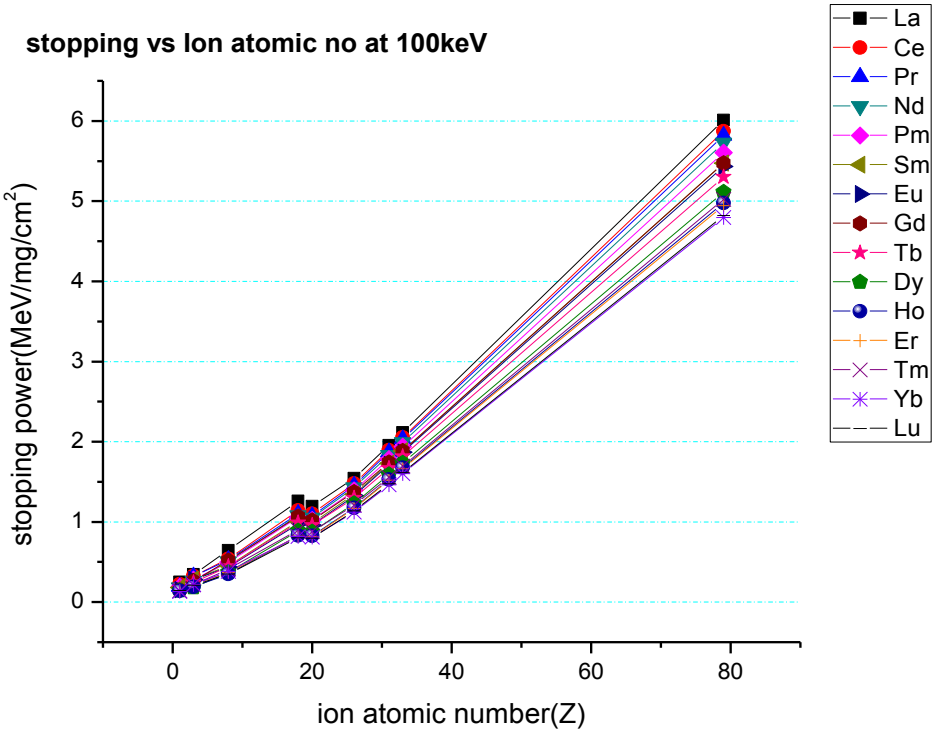


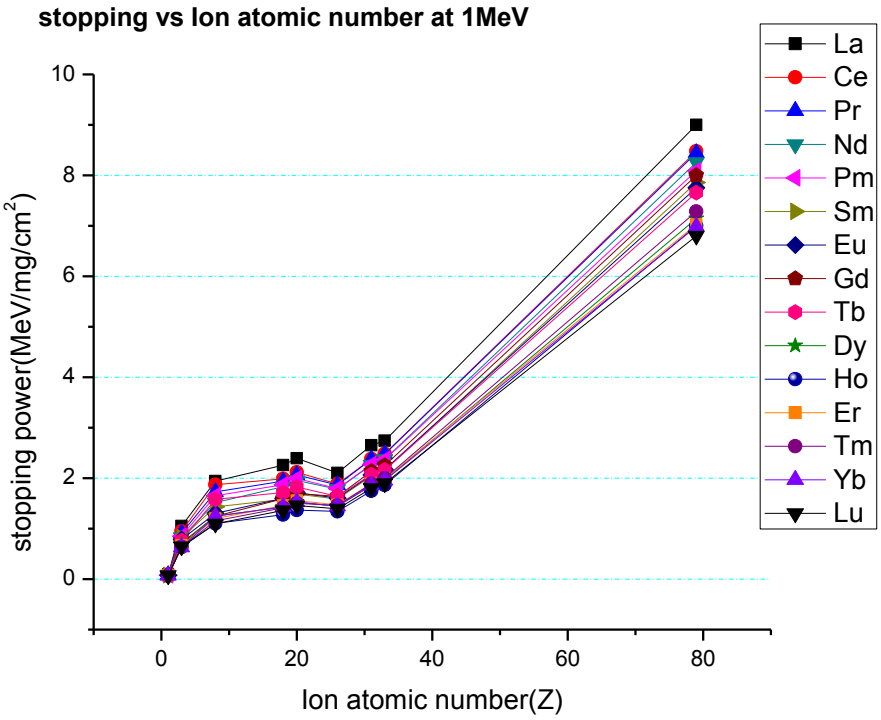
Fig4.15: Stopping of the different projectiles on each of the lanthanides

From the above plots we can see how the stopping increases with the increase in mass/atomic number of the ion. Stopping of all the ions follow a similar curve of reaching a peak and then gradually decreasing or stabilizing within the energy range taken, except for gold. There is a dip in the stopping in the stopping of gold near the 10MeV mark. Since gold has a high atomic mass the nuclear stopping in gold is very high and contributes to the total stopping in the lower energies. Therefore when it decreases the total stopping takes a dip as the electronic stopping is not high enough to compensate for the loss of nuclear stopping.

The next few plots depict the variation of stopping power with the mass/atomic number of the projectile ion. We can see that the increase in stopping is almost linear for all energies. However for different energies the slope of the graph may vary. Also it can be seen that the stopping decreases along with the progression of the elements in the lanthanide series i.e. the stopping in lanthanum is highest and it decreases to become the lowest in Lutetium.




stopping vs Ion atomic no at 100keV
stopping power(MeV/mg/cm2)
ion atomic number(Z)
0
1
2
3
4
5
6
0
20
40
60
80
La
Ce
Pr
Nd
Pm
Sm
Eu
Gd
Tb
Dy
Ho
Er
Tm
Yb
Lu


stopping vs Ion atomic number at 1MeV
stopping power(MeV/mg/cm2)
Ion atomic number(Z)
0
2
4
6
8
10
0
20
40
60
80
La
Ce
Pr
Nd
Pm
Sm
Eu
Gd
Tb
Dy
Ho
Er
Tm
Yb
Lu

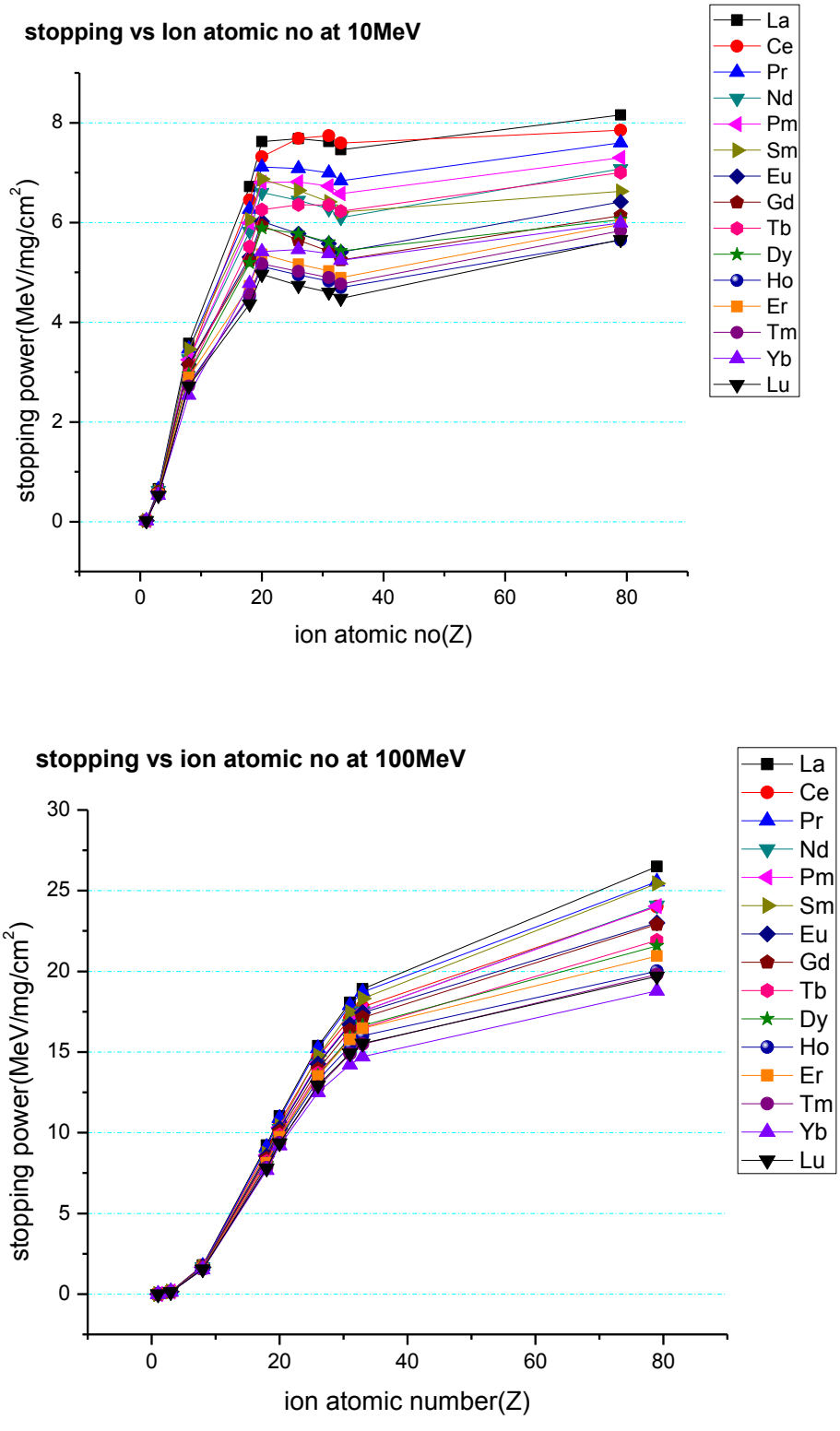


Fig4.16: variation of stopping with ion atomic number

Stopping of hydrogen in the lanthanide compounds

The following plots show the stopping of hydrogen ion in the lanthanide compounds Ce_2O_3, $GdBr_3$, $LaAlO_3$ and Pr_2S_3. The energy range has been taken from 10keV to 10MeV.

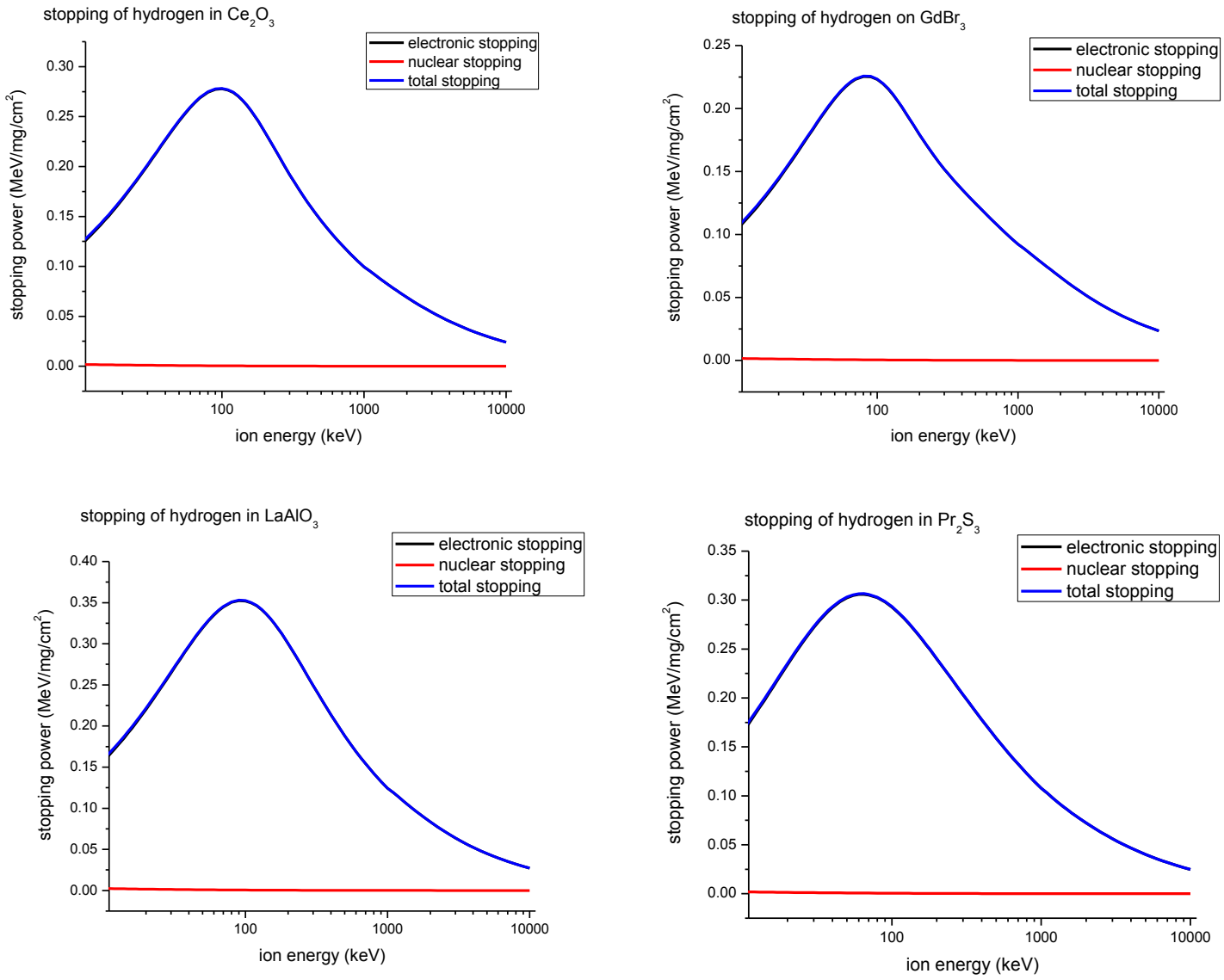


Fig 4.17: stopping of hydrogen in a few lanthanide compounds.

Similar to the stopping in elements the electronic stopping completely follows the total stopping. The nuclear stopping is very low and always remains lower than the electronic stopping. Its contribution to the total stopping is almost negligible The stopping increases till 100kev and then gradually decreases after.

Stopping of lithium in the lanthanide compounds

The following plots show the stopping of lithium ion in the lanthanide compounds Ce_2O_3, $GdBr_3$, $LaAlO_3$ and Pr_2S_3. The energy range has been taken from 10keV to 10MeV.

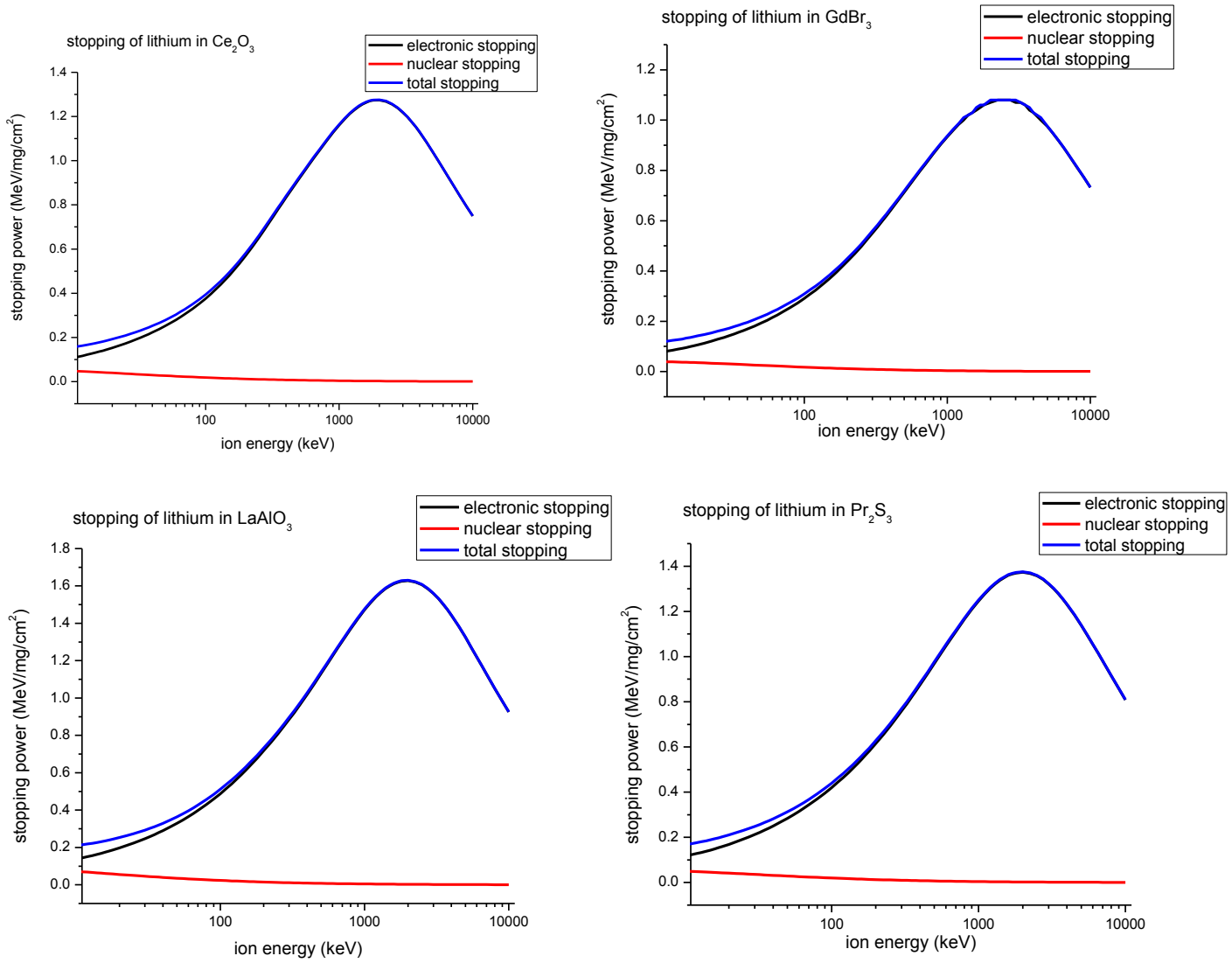


Fig4.18: stopping of lithium in a few lanthanide compounds

As in the case of hydrogen the nuclear stopping is always lower than the electronic stopping and it follows a decreasing trend. Its contribution to total stopping is very less. The electronic stopping follows the curve of total stopping except in lower energies (<<100keV). There is a gradual increase in the stopping till about 1MeV and then it decreases.

Stopping of oxygen ion in the lanthanide compounds.

The following plots show the stopping of oxygen ion in the lanthanide compounds Ce_2O_3, $GdBr_3$, $LaAlO_3$ and Pr_2S_3.

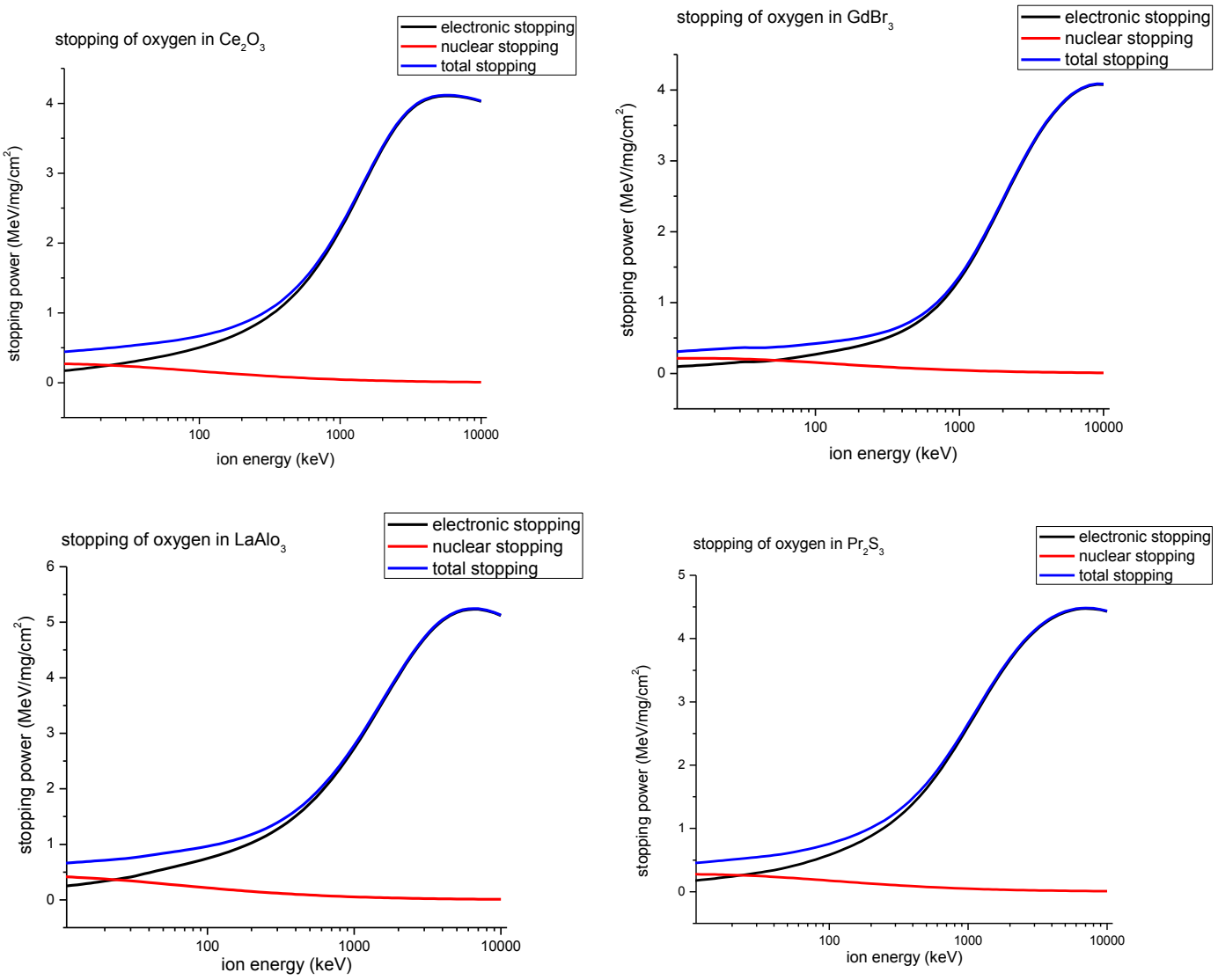


Fig 4.19: stopping of oxygen in lanthanide compounds

The nuclear stopping remains lower than electronic stopping except for very low energies around 10KeV. The electronic and total energy rise gradually till about 10MeV and then it follows a decreasing trend.

Stopping of Argon in the lanthanide compounds

The following plots show the stopping of argon ion in the lanthanide compounds Ce_2O_3, $GdBr_3$, $LaAlO_3$ and Pr_2S_3.

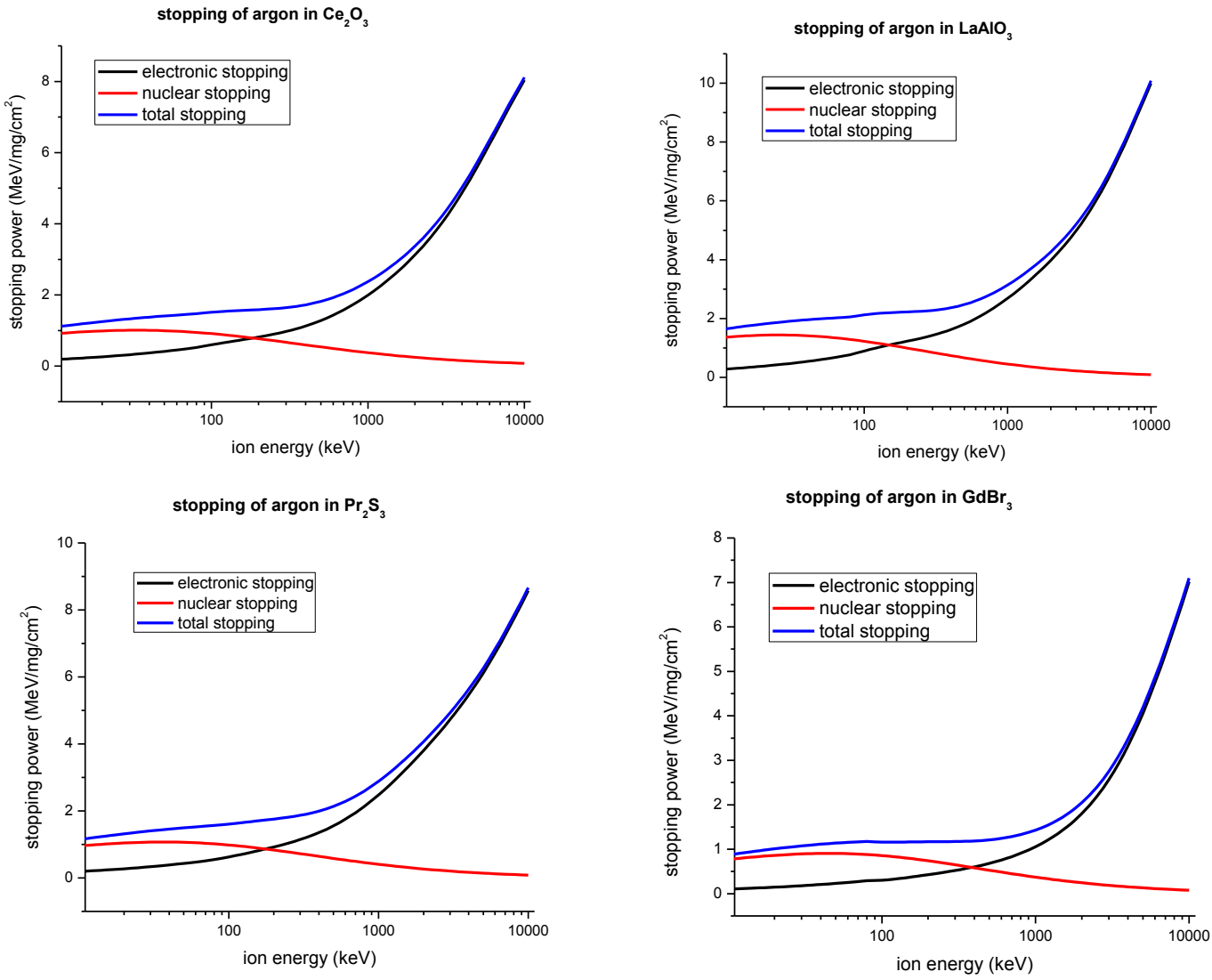


Fig4.20: stopping of argon in lanthanide compounds

The nuclear stopping is greater than electronic stopping at energies lower than 100KeV. It gradually decreases after 100KeV. The electronic stopping increases gradually. It follows the curve of total stopping after 1MeV. Before that the distinction between electronic stopping and total stopping is quite distinct. The peak lies beyond 10MeV.

Stopping of calcium in the lanthanide compounds

The following plots show the stopping of Calcium ion in the lanthanide compounds Ce_2O_3, $GdBr_3$, $LaAlO_3$ and Pr_2S_3.

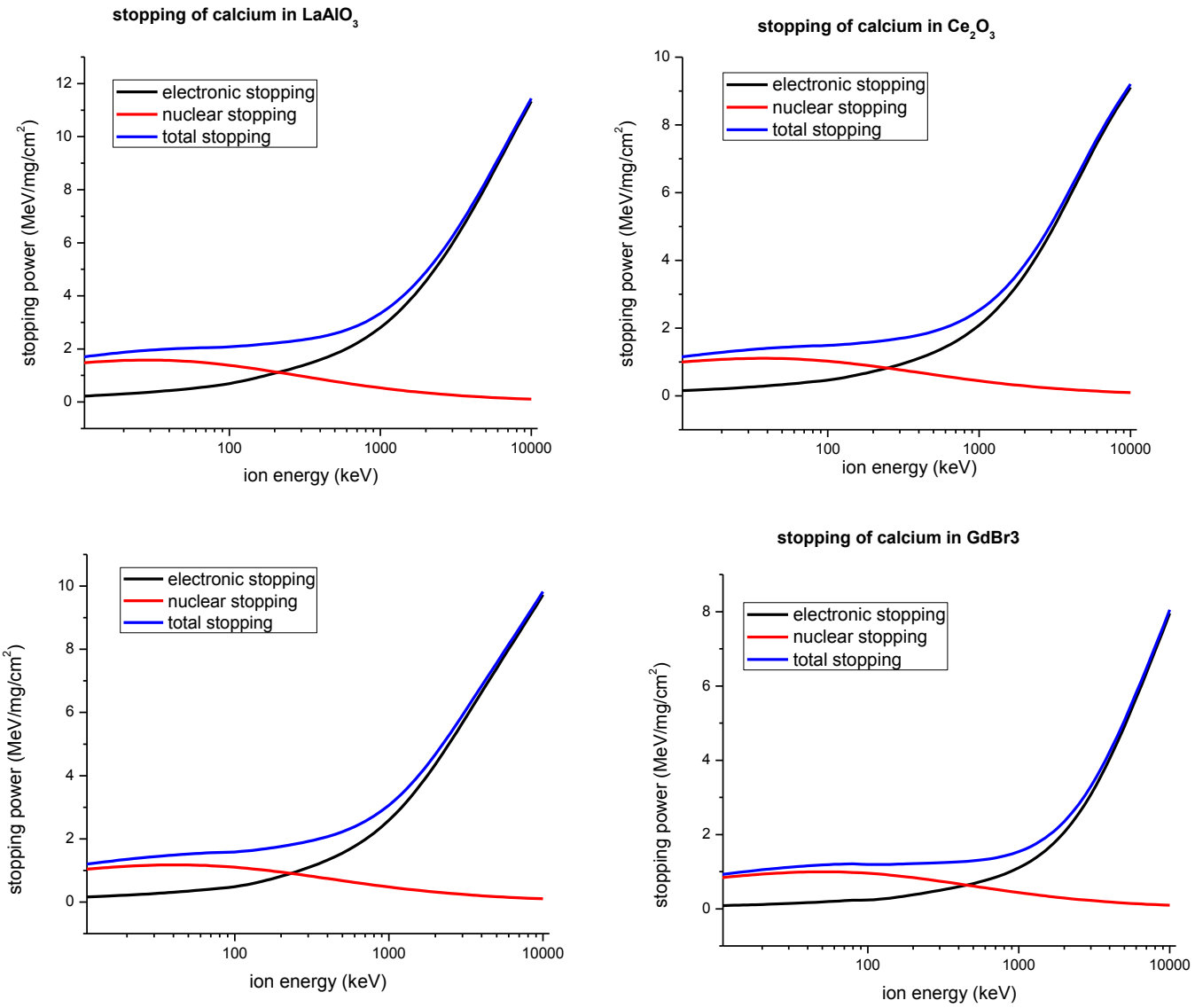


Fig4.21: stopping of calcium in lanthanide compounds

The nuclear stopping increases gradually till 100keV and then starts to decrease. It is greater than electronic stopping for energies lower than 100keV. Around approximately 200keV the nuclear stopping becomes less than electronic stopping. However this value increases to about 500keV in $GdBr_3$ indicating a variation with the increase in mass of the molecule. The electronic stopping increases steadily and the peak lies beyond 10MeV.

Stopping of iron in lanthanide compounds

The following plots show the stopping of iron ion in the lanthanide compounds Ce_2O_3, $GdBr_3$, $LaAlO_3$ and Pr_2S_3.

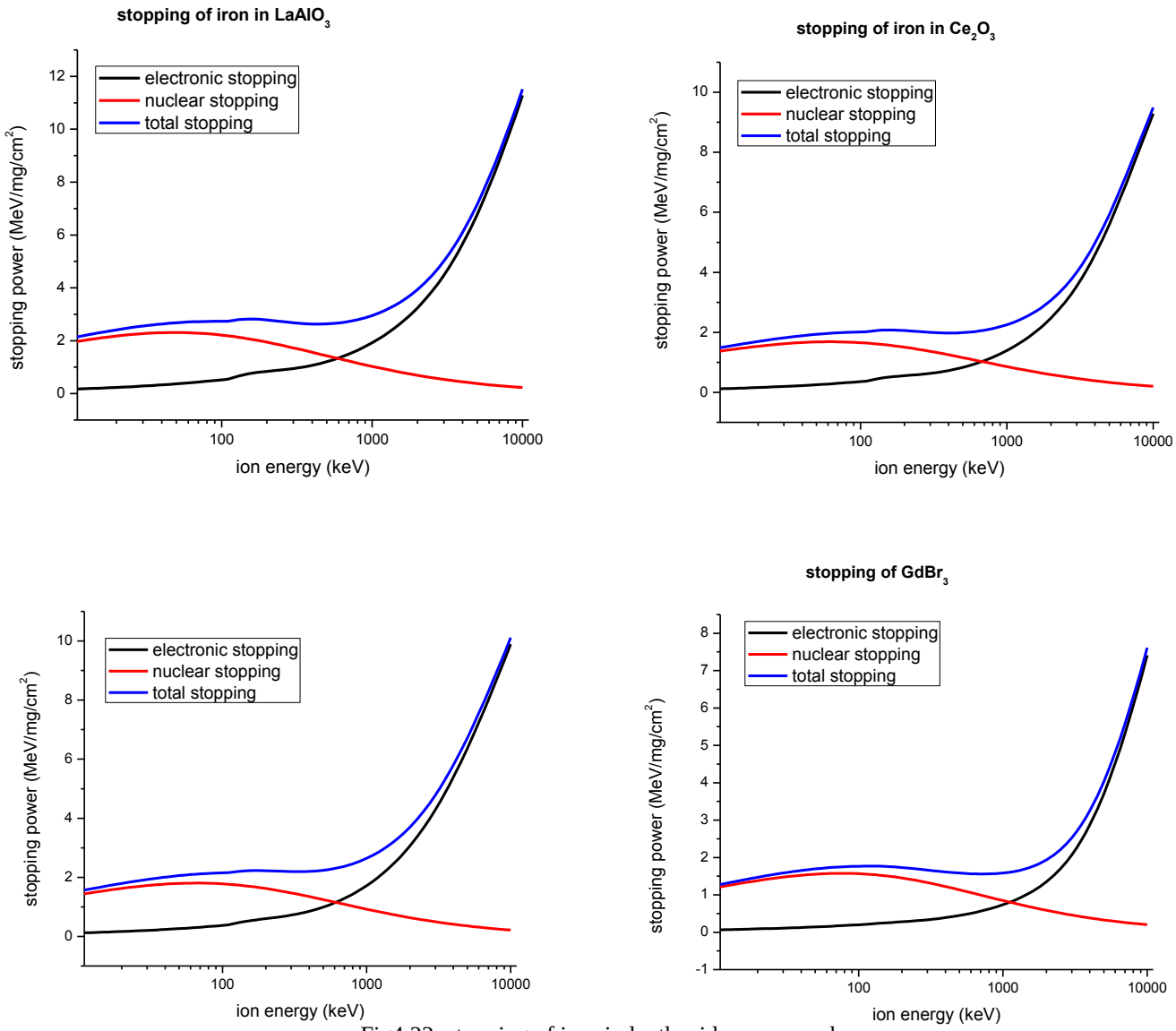


Fig4.22: stopping of iron in lanthanide compounds

The electronic stopping follows the curve of total stopping in high energies. Before 5MeV there is a distinct difference between the too. The electronic stopping curve gradually increases till 1Me after which the slope increases. Similarly the total energy increases gradually but experiences a dip around 1MeV. After the dip however it increases rapidly. The nuclear stopping is greater in lower energies but after around 1MeV it becomes less than electronic stopping.

Stopping of Gallium in Lanthanide compounds.

The following plots show the stopping of gallium ion in the lanthanide compounds Ce_2O_3, $GdBr_3$, $LaAlO_3$ and Pr_2S_3.

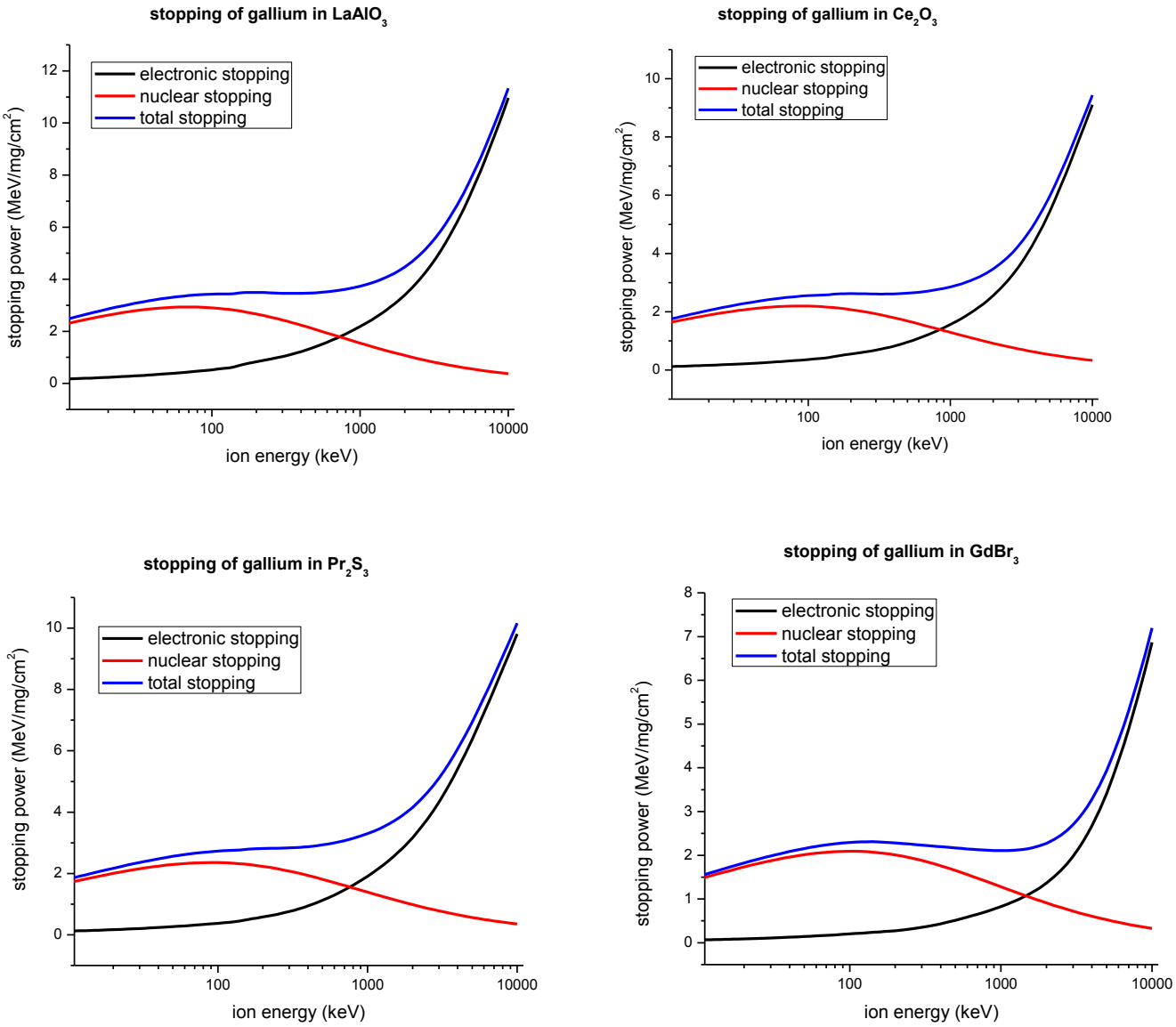


Fig4.23: stopping of Gallium in few lanthanide compounds

The nuclear stopping is significantly higher than electronic stopping in lower energies, however it decreases after 100keV and becomes less than electronic stopping between 1MeV to 2MeV. The electronic stopping has a gentle slope in lower energies but increases rapidly after 1MeV. The total energy experiences a dip near the 1MeV mark and then it increases rapidly.

Stopping of arsenic in lanthanide compounds

The following plots show the stopping of Arsenic ion in the lanthanide compounds Ce_2O_3, $GdBr_3$, $LaAlO_3$ and Pr_2S_3.

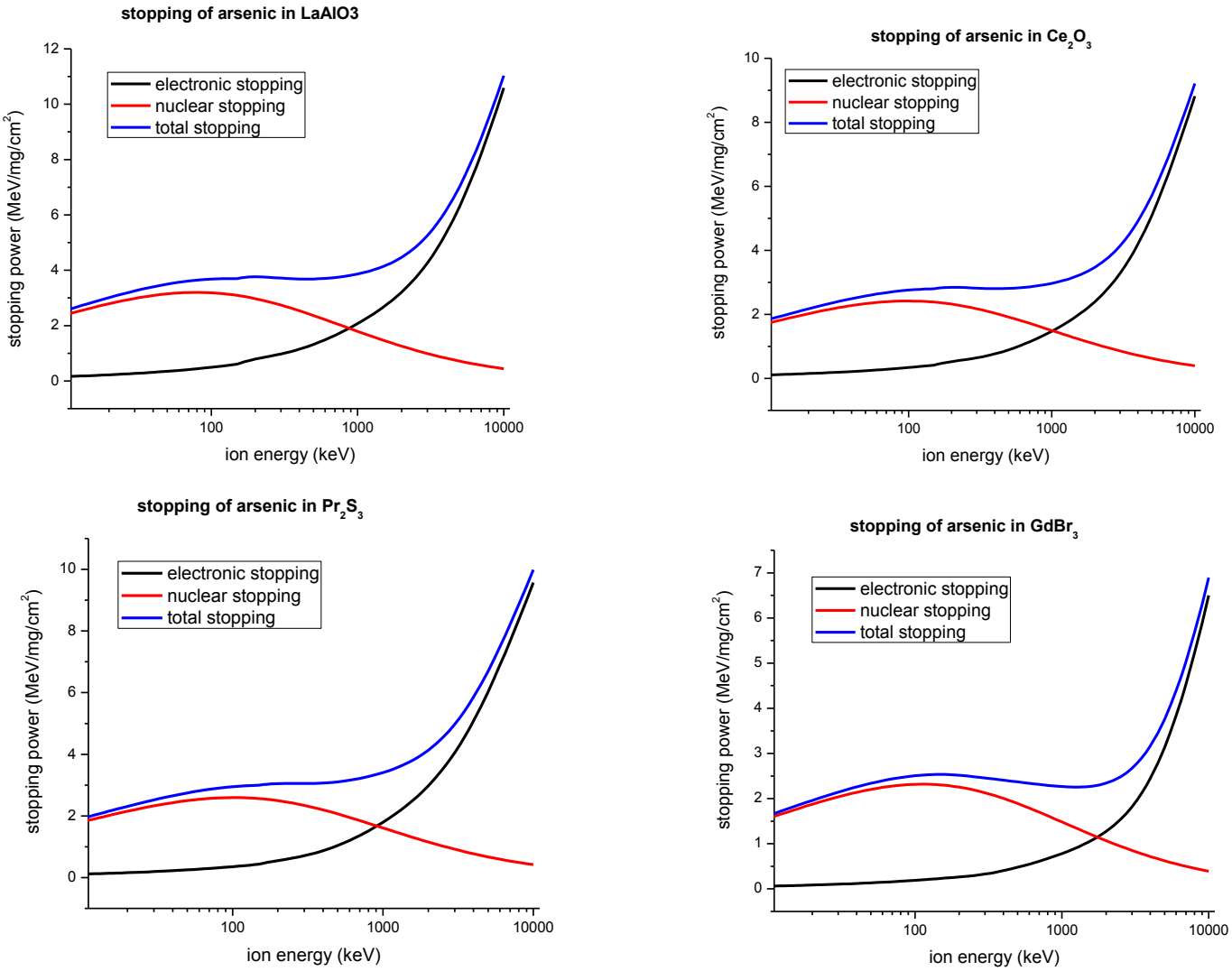


Fig4.24: stopping of arsenic in a few lanthanide compounds

The nuclear stopping is significantly greater in this case as compared to previous ions, but it decreases in higher energies and becomes less than the electronic stopping after 1MeV. The electronic stopping gradually increases in lower energies (<<1MeV) but there is a rapid increase after that. The total energy experiences a dip near 1MeV and then increases. The peak lies beyond 10MeV and there is a distinct difference between electronic stopping and total stopping throughout the plot.

Stopping of Gold in lanthanide compounds

The following plots show the stopping of gold in the lanthanide compounds Ce_2O_3, $GdBr_3$, $LaAlO_3$ and Pr_2S_3.

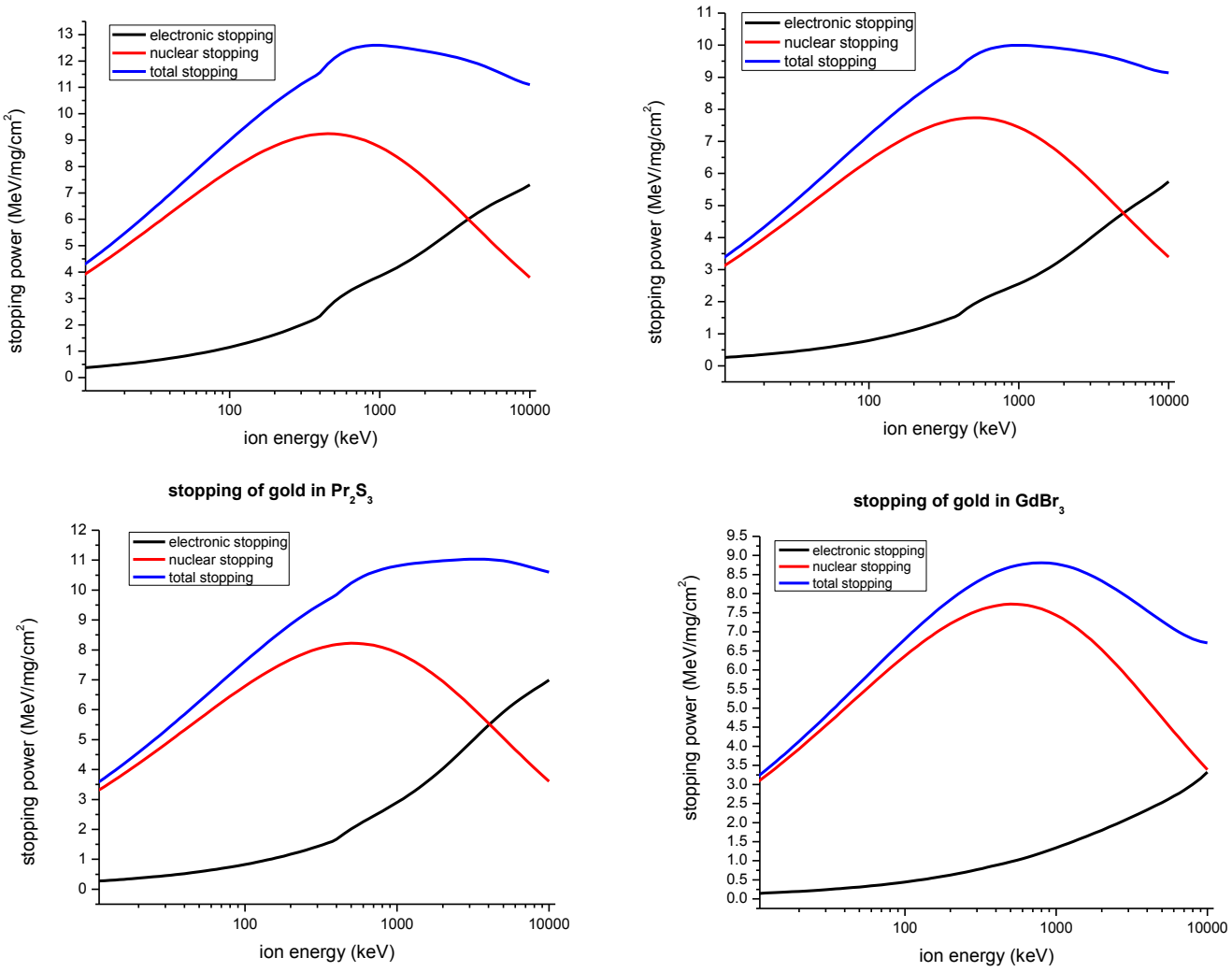


Fig4.25: stopping of gold in few lanthanide compounds

Unlike the previous ions, the electronic stopping in this case doesn't follow the curve of total stopping and there is a huge difference between the two. Nuclear stopping is high and correlates with the total stopping curve more in lower energies. However it starts to decrease around 1MeV. At around 4MeV it becomes less than the electronic stopping. For stopping in $GdBr_3$ this value is around 10MeV. The total stopping follows a decreasing trend after reaching a peak at 1MeV.

In the plots given below the stopping from the different ions are grouped together in each of the lanthanide compounds. It gives clear understanding of how the stopping varies for the different projectiles. The compounds used are as follows.

$LaAlO_3$ - Lanthanum aluminate

Ce_2O_3 – Cerium (III) oxide

Pr_2S_3 - Praseodymium(III) sulfide

Nd_2O_3 – Neodymium (III) oxide

$PmCl_3$ – Promethium(III) chloride

Sm_2O_3 – Samarium (III) oxide

Eu_2O_3 – Europium (III) oxide

$GdBr_3$ – Gadolinium(III) bromide

Tb_2O_3 – Terbium(III) oxide

Dy_2O_3 – Dysprosium(III) oxide

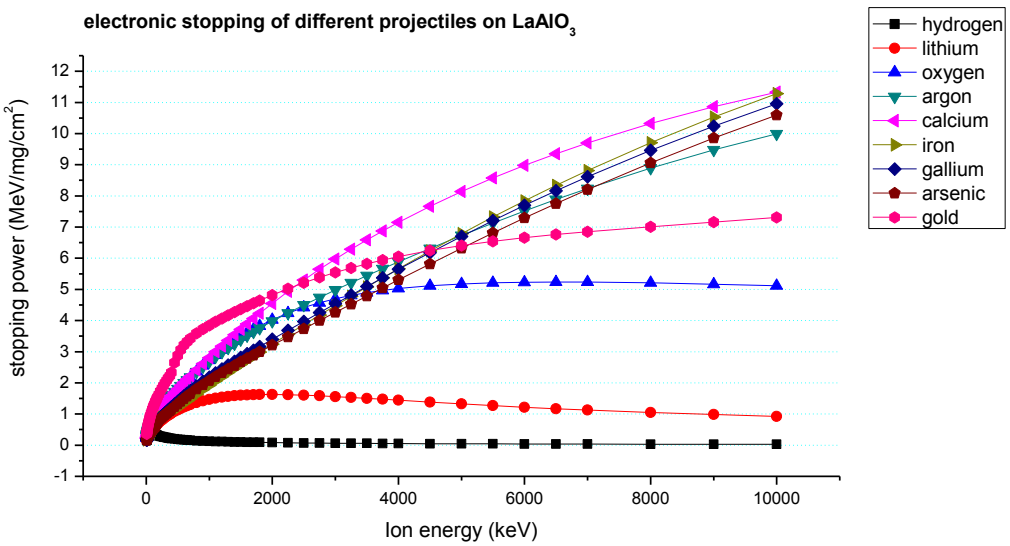
$HoBr_3$ – Holmium(III) bromide

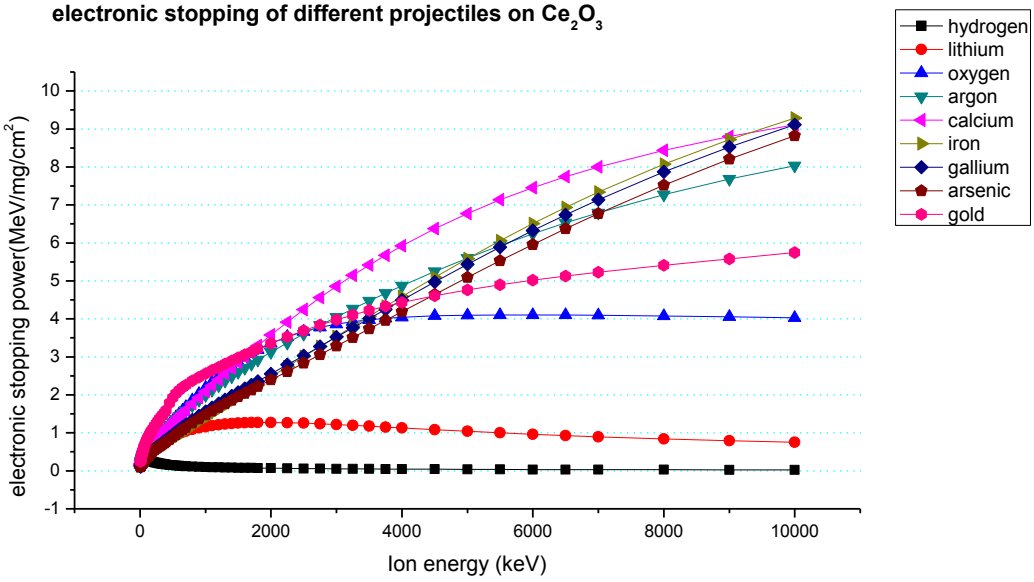
Er_2O_3 – Erbium(III) oxide

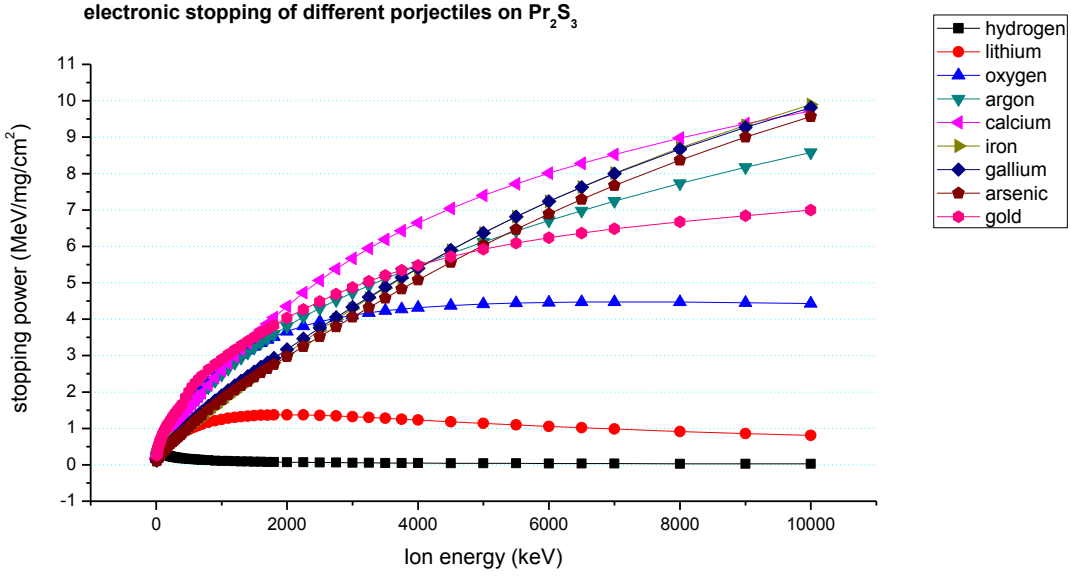
Tm_2O_3 – Thulium(III) oxide

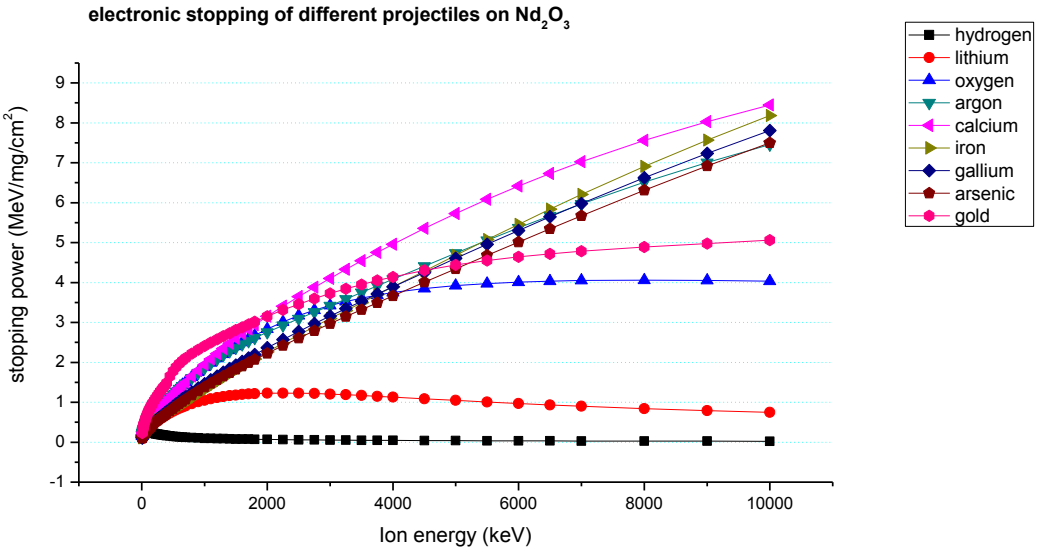
$YbCl_3$ – Ytterbium(III) chloride

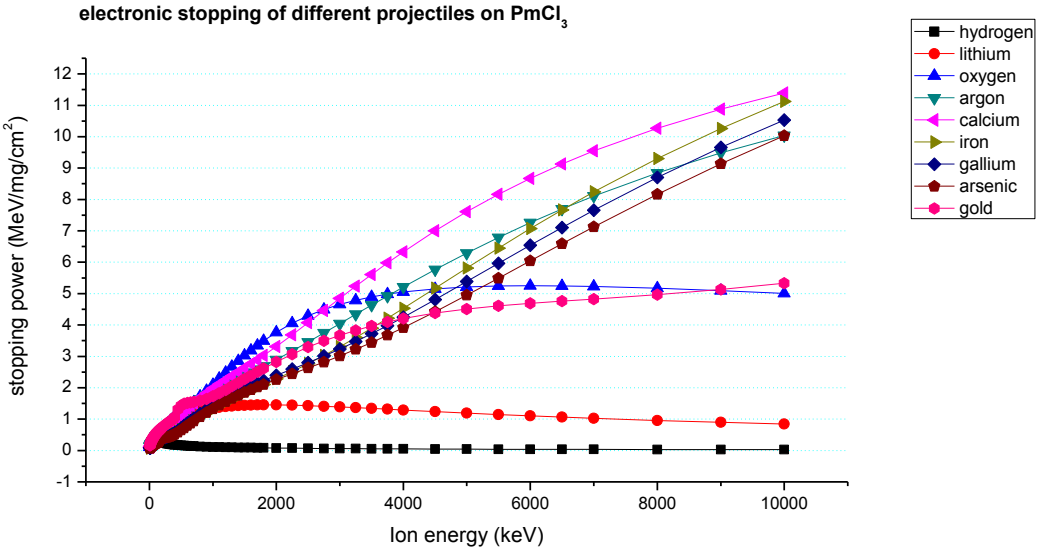
$LuCl_3$ – Lutetium(III) chloride

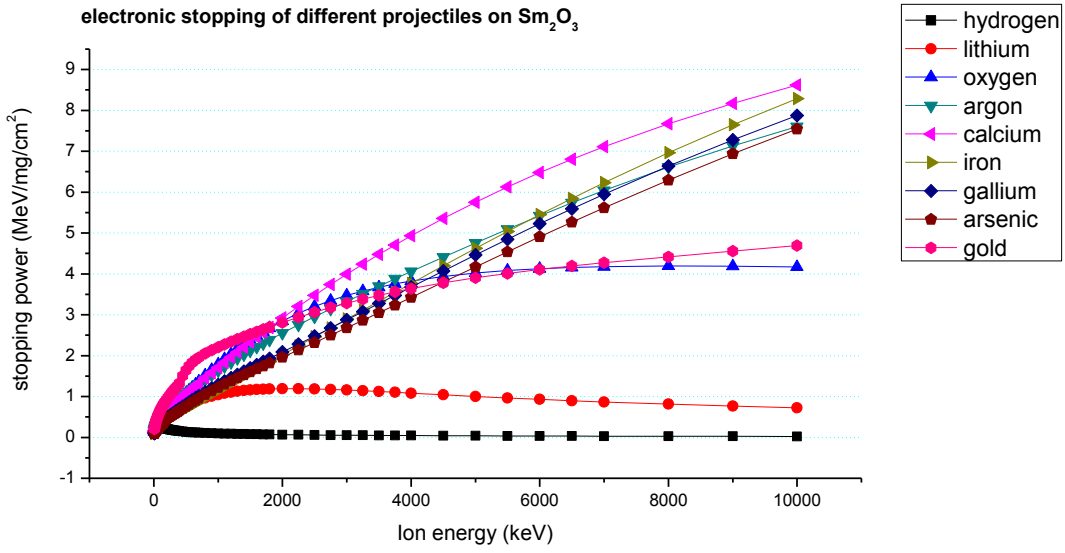

electronic stopping of different projectiles on LaAlO3
stopping power (MeV/mg/cm2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold

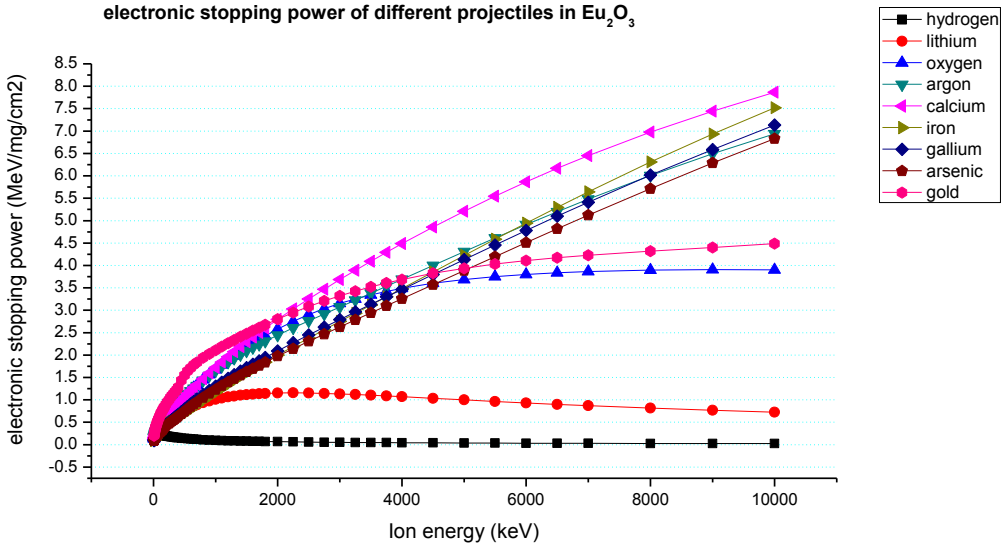

electronic stopping of different projectiles on Ce2O3
electronic stopping power(MeV/mg/cm2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold

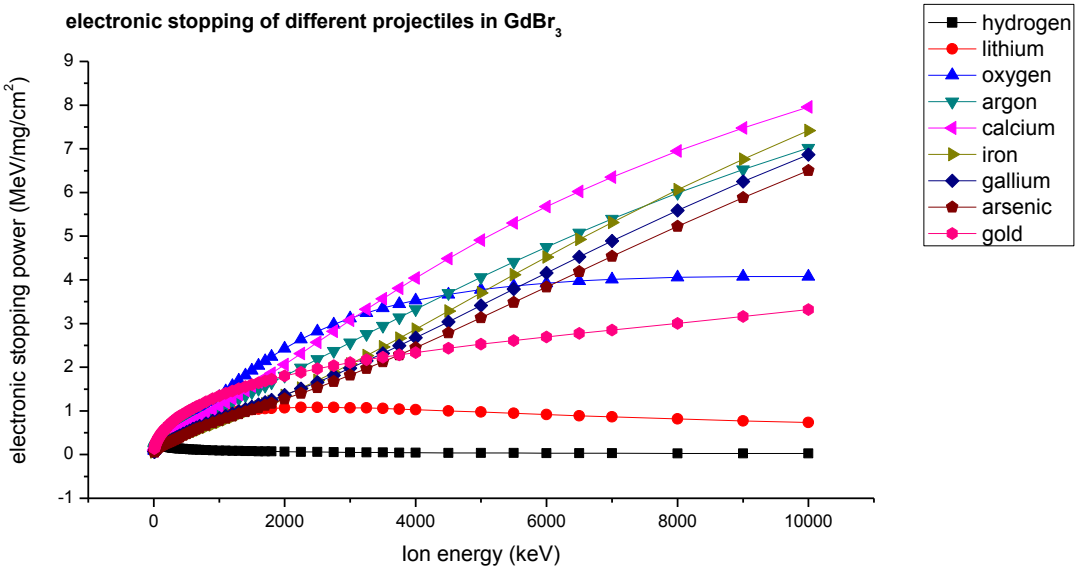

electronic stopping of different porjectiles on Pr2S3
stopping power (MeV/mg/cm2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold

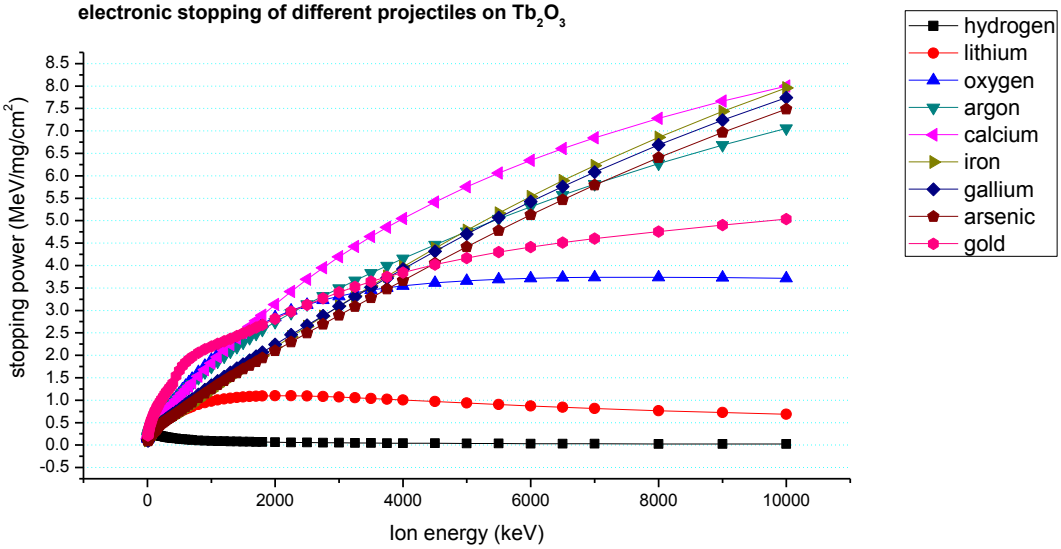

electronic stopping of different projectiles on Nd_2O_3
stopping power (MeV/mg/cm^2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold

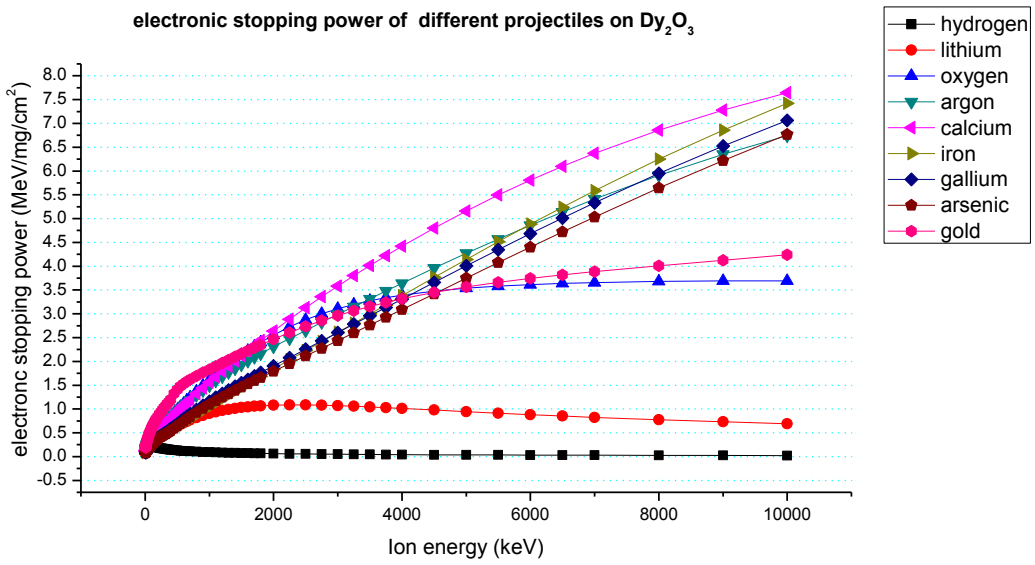

electronic stopping of different projectiles on $PmCl_3$
stopping power (MeV/mg/cm^2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold

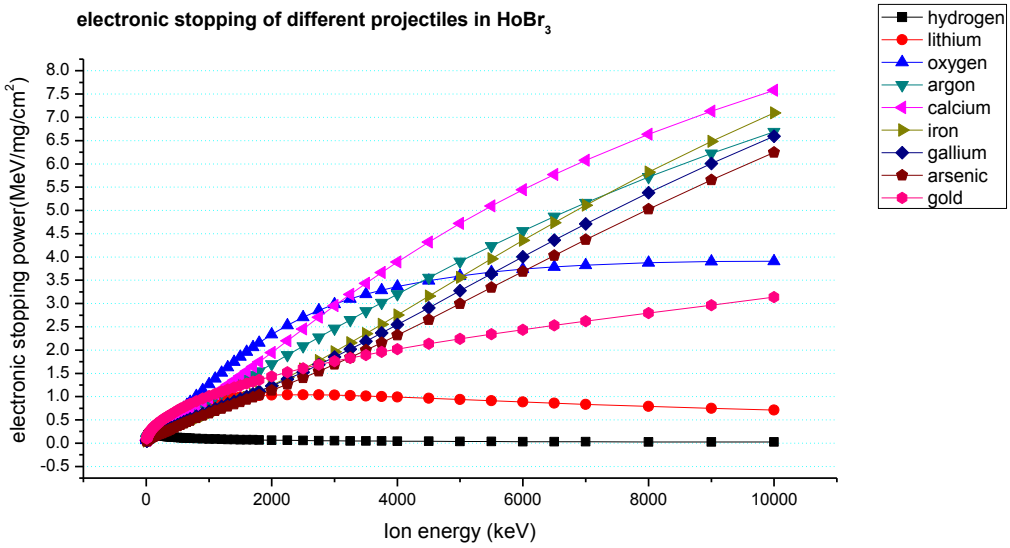

electronic stopping of different projectiles on Sm_2O_3
stopping power (MeV/mg/cm^2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold

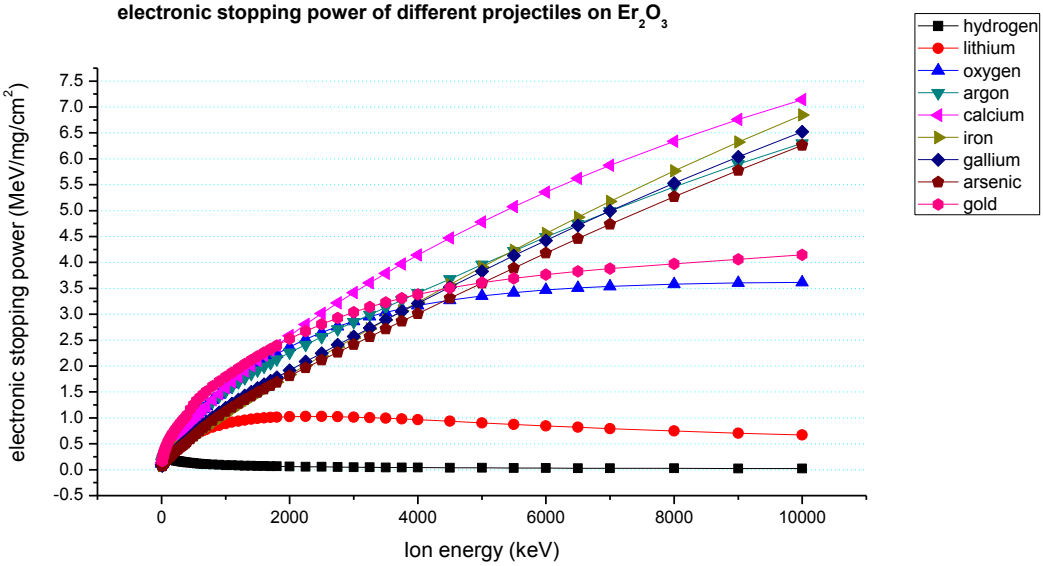

electronic stopping power of different projectiles in Eu_2O_3
electronic stopping power (MeV/mg/cm2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


electronic stopping of different projectiles in $GdBr_3$
electronic stopping power (MeV/mg/cm^2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


electronic stopping of different projectiles on Tb_2O_3
stopping power (MeV/mg/cm^2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


electronic stopping power of different projectiles on Dy_2O_3
electronc stopping power (MeV/mg/cm^2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


electronic stopping of different projectiles in $HoBr_3$
electronic stopping power(MeV/mg/cm^2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


electronic stopping power of different projectiles on Er_2O_3
electronic stopping power (MeV/mg/cm^2)
Ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold

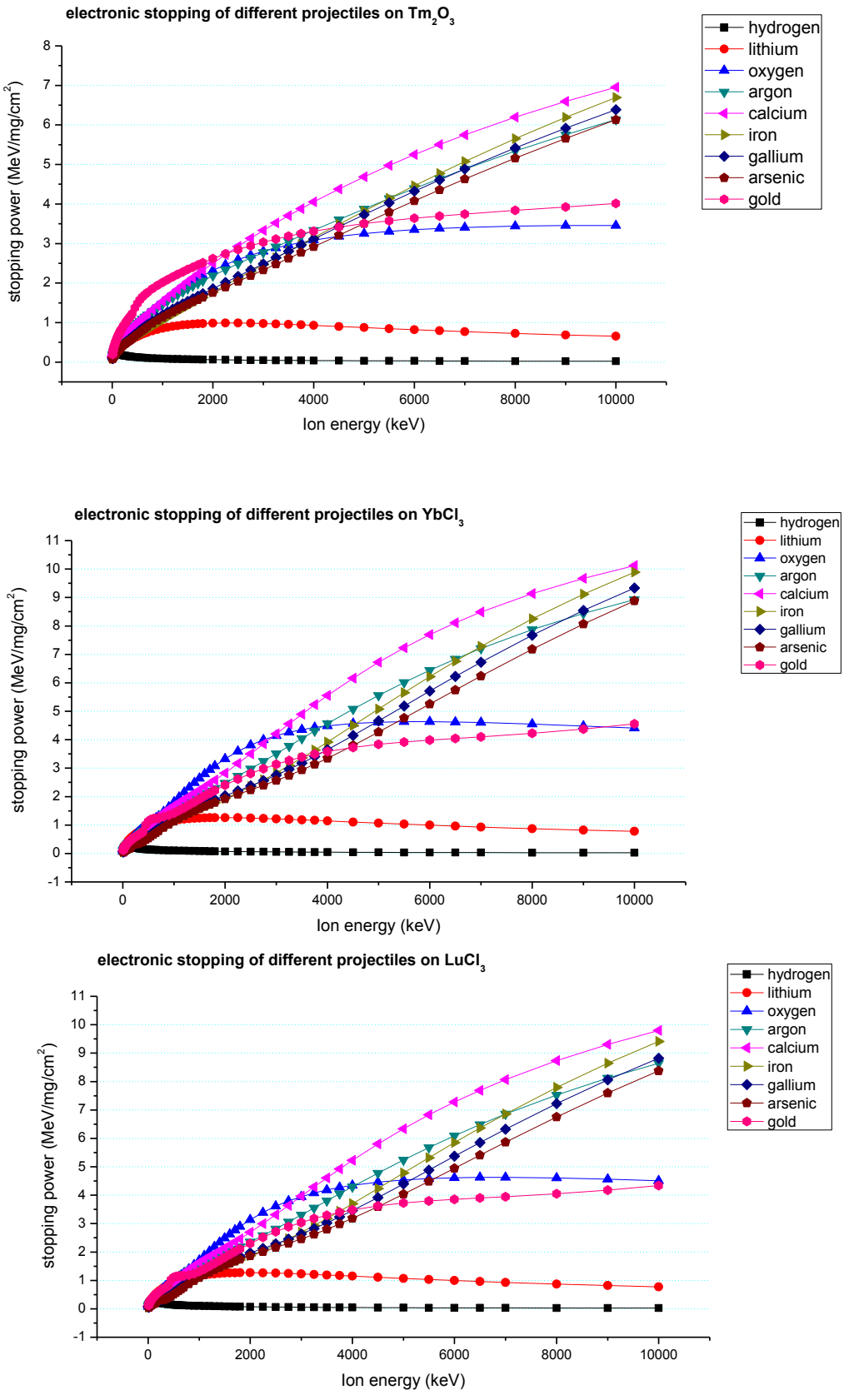
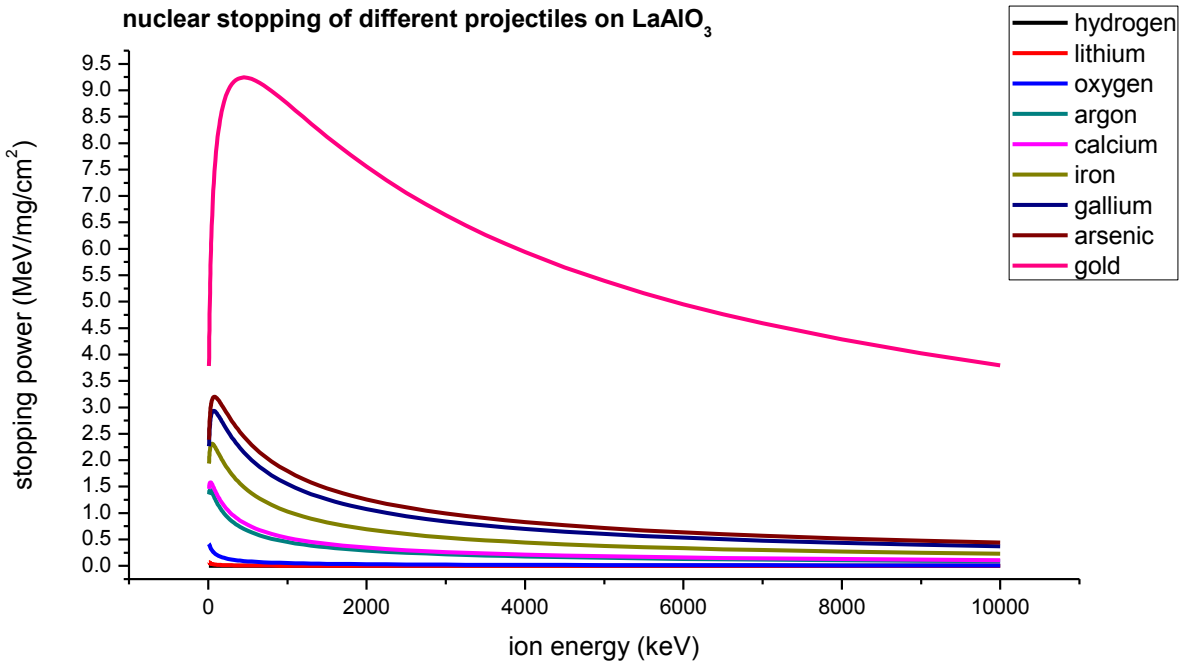
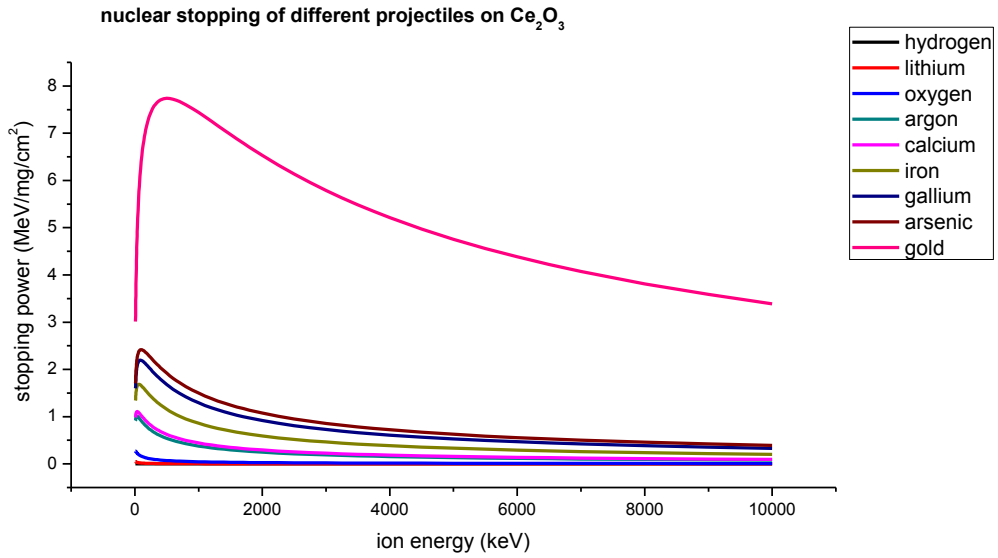


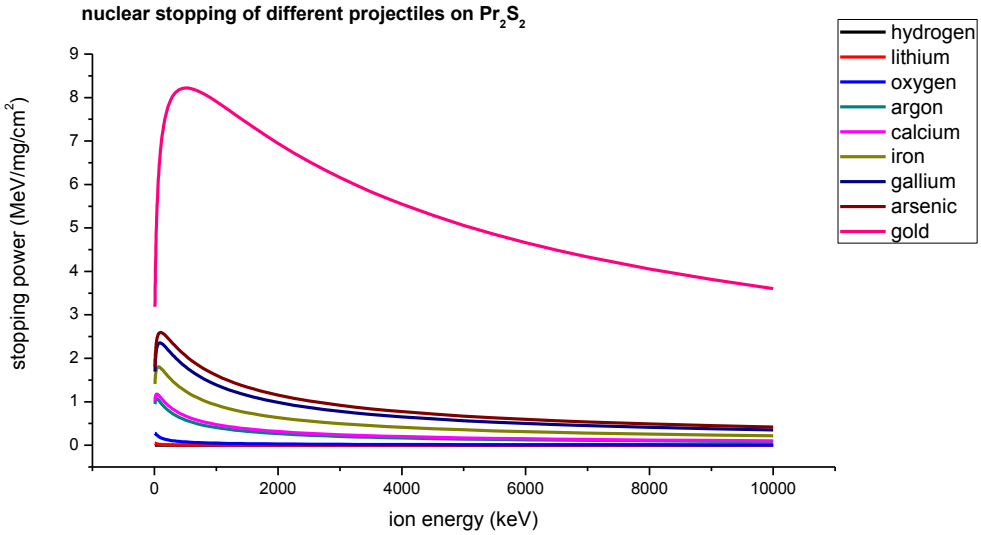
Fig4.26: stopping of different projectiles in lanthanide compounds

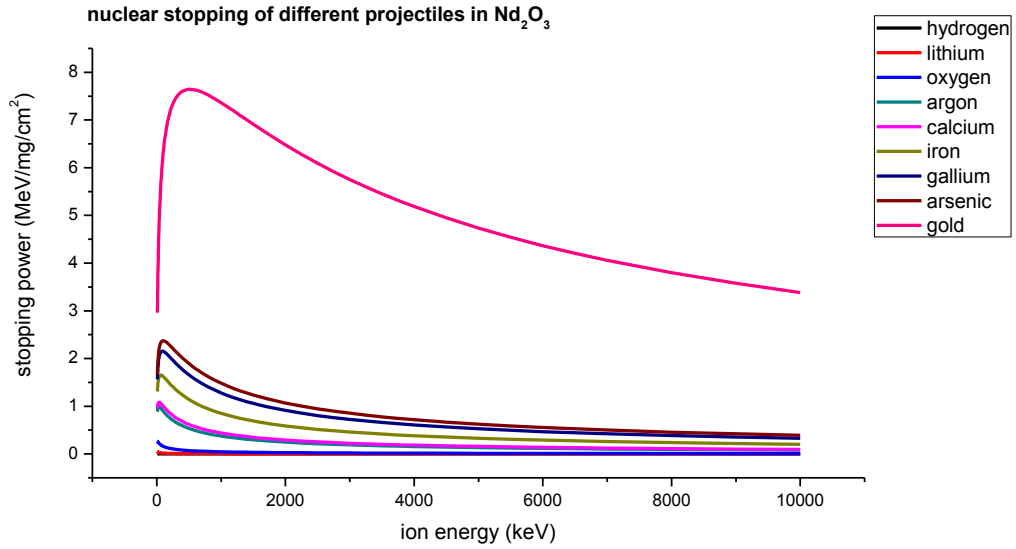
The stopping follows a general trend of rapidly increasing in the lower energies and then there is a steady increase for higher energies. The overall stopping power first increases with the mass of the ion and then it decreases. We can see from the plots that the stopping is maximum for calcium and then it decreases. The stopping of gold and oxygen is almost comparable, even though the mass of gold is much higher than that of oxygen. Another observation that can be made from the plots is that the stopping shows a decrease in value with the increase in molecular mass of the target compound i.e. for compounds with higher molecular mass the stopping is lower as compared to compounds with lower molecular mass. For example the molecular mass of $LaAlO_3$ is lowest at 213.89g/mol but the values of the stopping power is more in this case as compared to the other compounds.

The following graphs plot the nuclear stopping in each of the compounds. The stopping due to all the projectile ions are grouped together.




nuclear stopping of different projectiles on Ce_2O_3
stopping power (MeV/mg/cm^2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


nuclear stopping of different projectiles on Pr_2S_2
stopping power (MeV/mg/cm^2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold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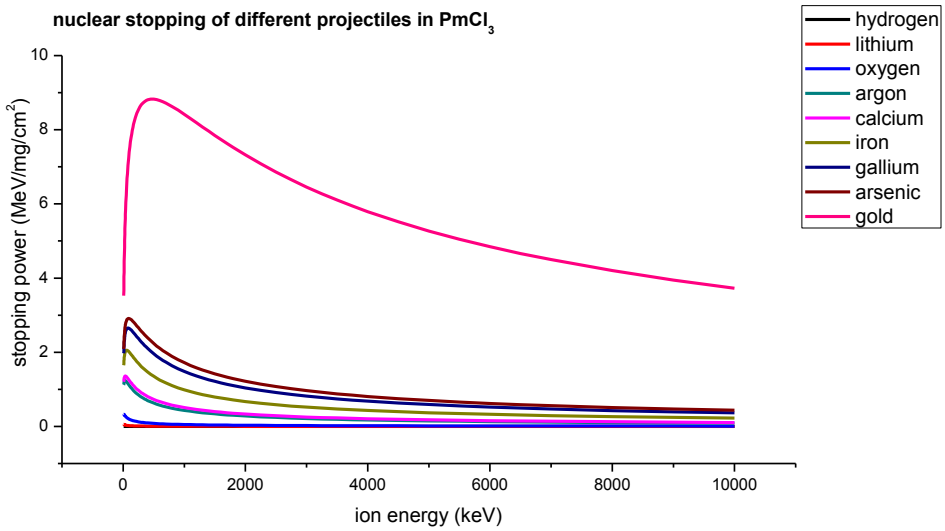
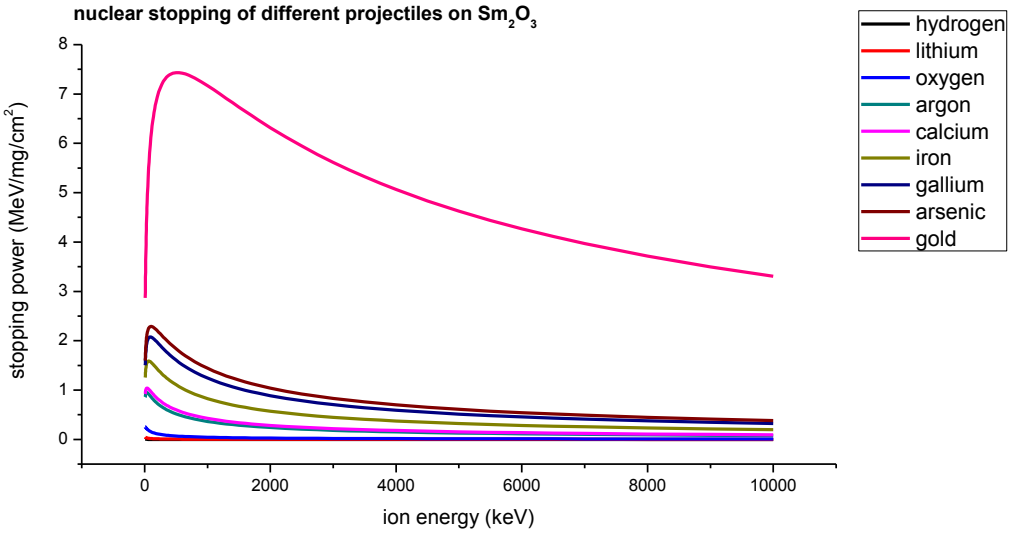
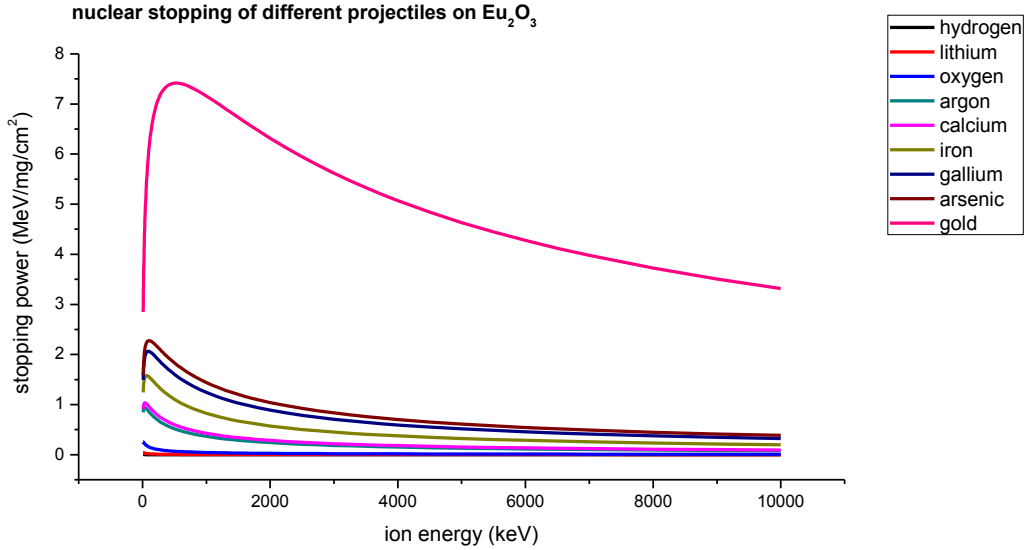
stopping power (MeV/mg/cm^2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


nuclear stopping of different projectiles in PmCl3
stopping power (MeV/mg/cm2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


nuclear stopping of different projectiles on Sm2O3
stopping power (MeV/mg/cm2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold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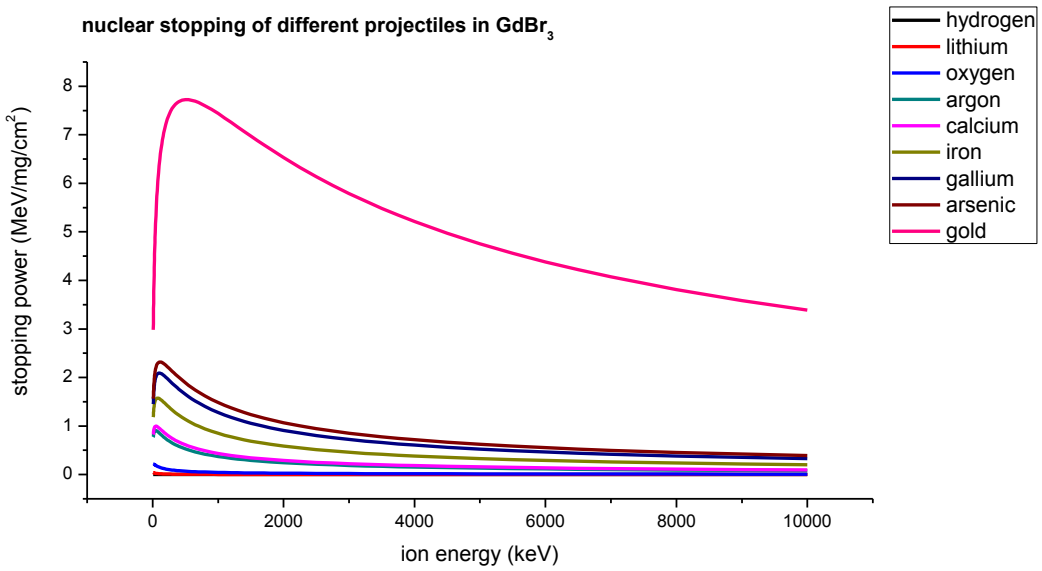
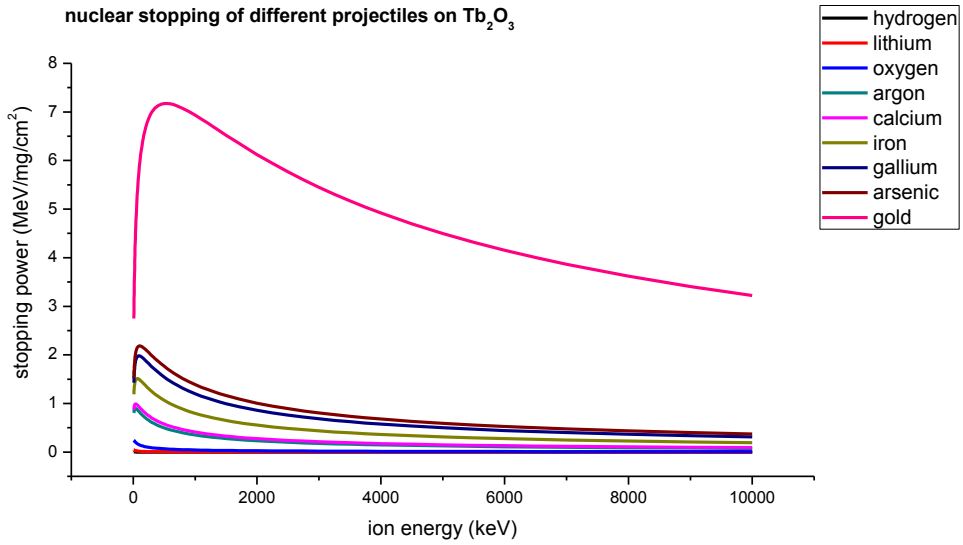
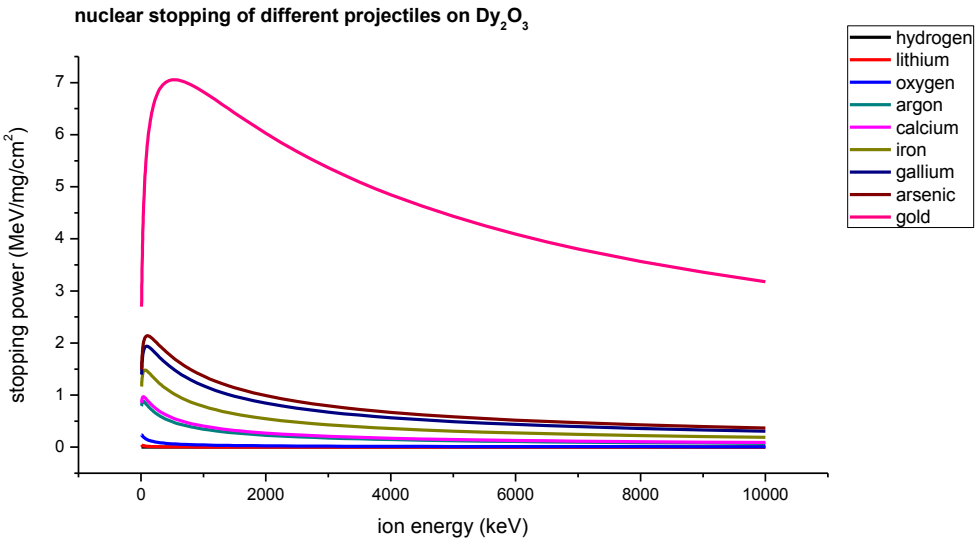
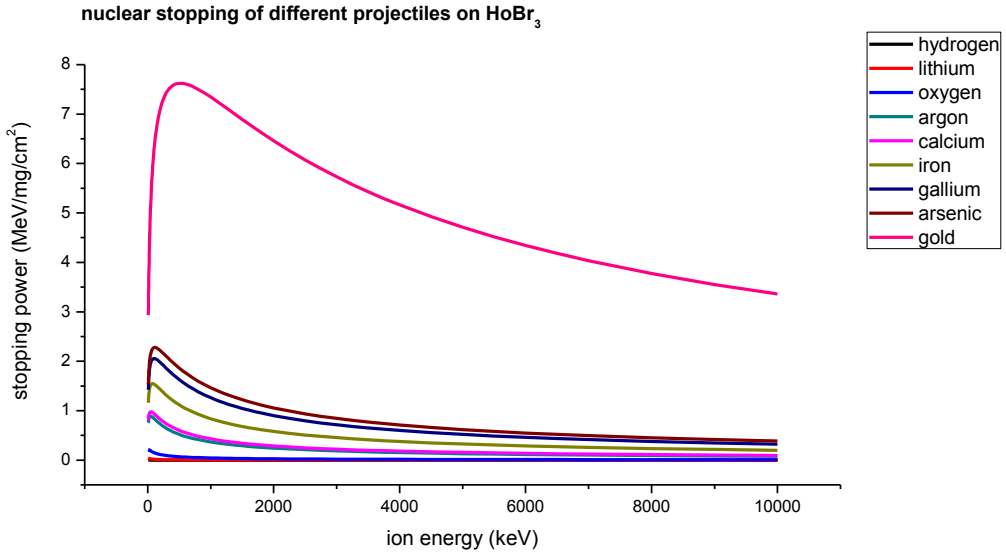
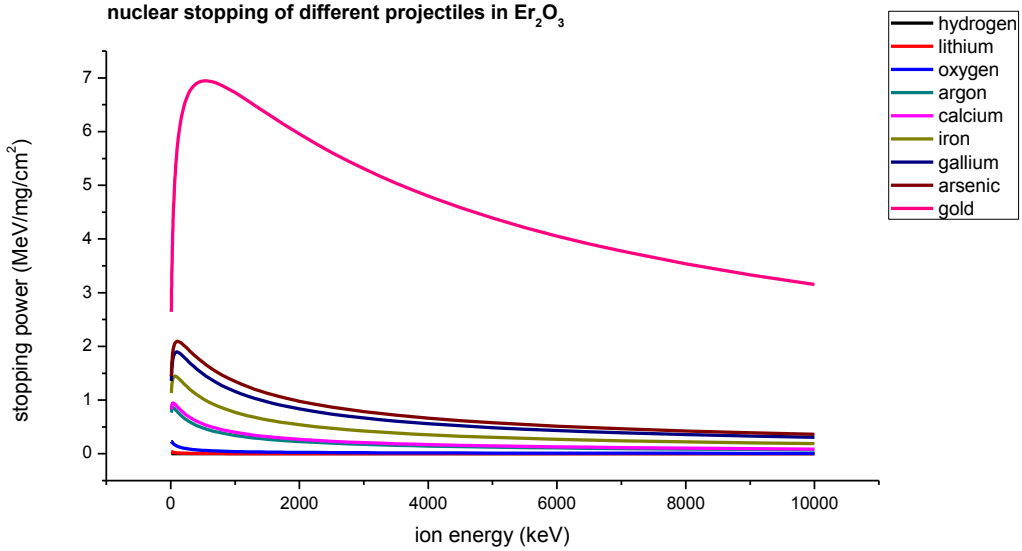
stopping power (MeV/mg/cm2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold

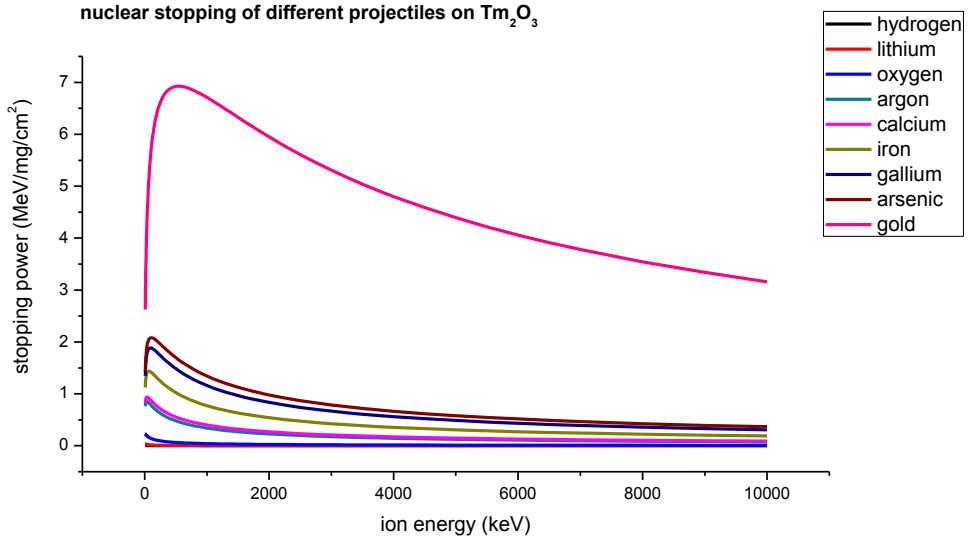

nuclear stopping of different projectiles in GdBr3
stopping power (MeV/mg/cm2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


nuclear stopping of different projectiles on Tb2O3
stopping power (MeV/mg/cm2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


nuclear stopping of different projectiles on Dy2O3
stopping power (MeV/mg/cm2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


nuclear stopping of different projectiles on HoBr3
stopping power (MeV/mg/cm2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


nuclear stopping of different projectiles in Er2O3
stopping power (MeV/mg/cm2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold


nuclear stopping of different projectiles on Tm2O3
stopping power (MeV/mg/cm2)
ion energy (keV)
hydrogen
lithium
oxygen
argon
calcium
iron
gallium
arsenic
gold

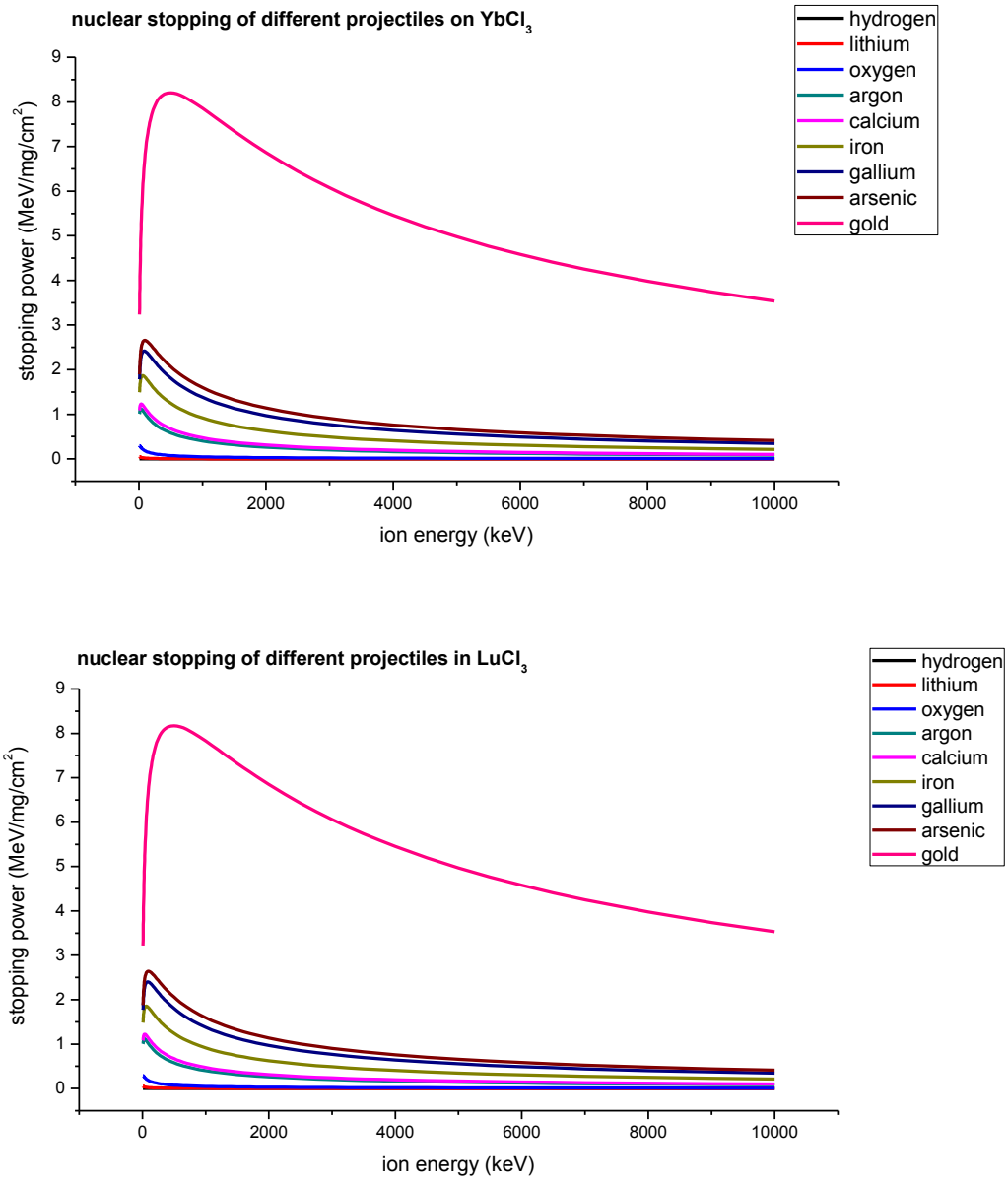


Fig4.27: nuclear stopping of different projectiles in compounds of lanthanides.

From the above plots it is evident that nuclear stopping is very low compared to electronic stopping and it is very low as in higher energies. The nuclear stopping reaches a peak rapidly and then decreases gradually. Most of the peaks that are reached by the ions lie before 1MeV. Also the nuclear stopping remains lower than electronic stopping for light ions like hydrogen and lithium slowing down in heavy materials. The nuclear stopping also increases with the mass of the ion. Here we can see that gold has the maximum nuclear stopping and also it is very large as compared to the other ions as gold has the largest mass/atomic number.

CHAPTER 5

SUMMARY AND CONCLUSIONS

The interest on the stopping power has been prevalent throughout the last century and is based on many applications in materials science, radiation physics and radiation shielding, nuclear medicine and ion implantation techniques. The slowing down of charged particles in matter can be represented by the Bragg's curve which describes the force as a function of the target depth. This curve is of high practical importance in radiation therapy. Stopping of particles is also a very important aspect in ion implantation. Atoms of the solid are removed from their lattice positions when they receive significant recoil energies when struck by the ion. This produces a cascade of further collisions in the material. Damage production during ion implantation in metals and semiconductors are caused by these collisions. Nuclear stopping refers to the mean energy loss occurring at all possible scattering angles. At low energies the probability for elastic scattering is considerably high, so nuclear stopping at low energies, contribute significantly to the total stopping power and in some cases, even exceed the electronic stopping. For light ions travelling in heavy solids however the nuclear stopping always remain lower than the electronic stopping. Also as the mass of the incoming ion increases the probability of elastic collisions increase hence the nuclear stopping increases as we see in the case of gold above. The stopping of ions in compounds may be different from the weighted stopping of ions in the elemental matter which makes up the compounds. This occurs in part because the outer shell electrons (which absorb much of the energy loss of slow ions) have different orbitals in the compound than they have in elemental matter. The difference in energy loss may be calculated using what is called the "Core and Bond" approximation. This approach separates out the stopping contributions from the binding electrons (bonds) from inner shell electrons (core), then alters the stopping for the bonding electrons based on the bonds found in the compound. However for compounds containing heavy atoms, Al (13) or greater, the difference is almost negligible. All experiments that are conducted in SRIM with compounds such as Al_2O_3, SiO_2, Fe_2O_3, Fe_3O_4, Si_3N_4 and many more, show less than 2% deviation from Bragg's rule which estimates the stopping by the sum of the stopping in the elemental constituents. That is, the stopping in Al_2O_3 is the same as the sum of the stopping in 2 Al + 3 O target atoms.

Computer simulation programs which depict the motion of ions through matter have been in development since 1960s. In these programs, the interaction of the ion with the nuclei in an elastic collision is done and the electronic stopping power is represented as a frictional force acting on the ion. In this work the SRIM software package is used to calculate the motion of the ions through the lanthanides. SRIM uses the very conventional BCA (binary collision approximation) method to calculate ion ranges and stopping. BCA treats the motion of an ion as series of individual collisions. SRIM provides reliable and accurate results of stopping power for various ion target combinations. However the BCA methods face some obstacles for describing the slowing down process of energetic ions realistically as basic assumption that collisions are binary results in severe problems when trying to take multiple interactions into account. SRIM also doesn't take the crystal structure into account. The best reliability in BCA is obtained by including multiple collisions in the calculations, which is a difficult task. Other programs like MARLOWE, BCCRYS and crystal-TRIM overcome these problems. A fundamentally more straightforward way to model multiple atomic collisions is provided by molecular dynamics (MD) simulations, in which the time evolution of a system of atoms is calculated by solving the equations of motion numerically.

The lanthanides are an interesting group of elements with various applications in research as well as medical fields. Lanthanide elements are used in superconductors, samarium-cobalt and neodymium-iron-boron high-flux rare-earth magnets, magnesium alloys, electronic polishers, refining catalysts and hybrid car components (primarily batteries and magnets). Lanthanides have replaced the hazardous thorium and their oxides are mixed with tungsten to improve their high temperature properties for TIG welding. Defense-related products like rangefinders and night vision goggles use lanthanide elements. The SPY-1 radar used in some Aegis equipped warships, and the hybrid propulsion system of *Arleigh Burke*-class destroyers all use rare earth magnets in critical capacities. Currently there is research showing that lanthanides elements can be used as anticancer agents. The main role of the lanthanides in these studies is to inhibit proliferation of the cancer cells. One of the specific elements from the lanthanide group that has been tested and used is cerium (Ce). There have been studies that use a protein-cerium complex

to observe the effect of cerium on the cancer cells. Another specific element that has been tested and used as an anti-cancer agent is lanthanum, more specifically lanthanum chloride ($LaCl_3$). When the lanthanum ion was introduced to the cell in vivo or in vitro, it inhibited the rapid growth and induced apoptosis of the cancer cells (specifically cervical cancer cells). Hence the knowledge of the behavior of lanthanides with different interactions become of utmost importance. This work is an attempt to study the behavior of different charged particles passing through the lanthanide elements and their compounds. A comparative study of the stopping power in lanthanides and how they vary along with different parameters like atomic mass, number and energy has been done. From this comparative analysis, it can be concluded that the stopping power values provide valuable information which can play an important role in analyses of these material and their different applications. It also gives an insight on the behavior of different projectiles in their passage through lanthanide materials, thus opening up provisions for more work in this aspect. The main challenge faced in this work has being lack of sufficient experimental data for the selected target materials within the energy range used for effective comparison with the theoretical values. Therefore it calls for more investigation into the lanthanide elements and their compounds. It would help to predict their behavior more accurately.

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