Project Presentation

TITLE

CALCULATION OF TIME OF FLIGHT USING TOFMS techniques

Out line of my talk

- What is mass spectrometry
- What is TOFMS
- Basic geometry of TOFMS
- Principle of TOFMS
- Total Time for the ion
- C-Programming for TOF
- Program for drawing Histogram
- Histogram
- Advantage of TOF
- Application

What is Mass Spectrometry?

Mass spectrometry is a powerful analytical technique that is used to identify unknown compounds, to quantify known compounds, and to elucidate the structure and chemical properties of molecules. - ASMS

Mass spectrometry (MS) is an analytical technique for the determination of the elemental composition of a sample or molecule. It is also used for elucidating the chemical structures of molecules, such as peptides and other chemical compounds. - Wikipedia

(Physics / General Physics) an analytical instrument in which ions, produced from a sample, are separated by electric or magnetic fields according to their ratios of charge to mass. A record is produced (mass spectrum) of the types of ion present and their relative amounts. – FreeDictionary.com

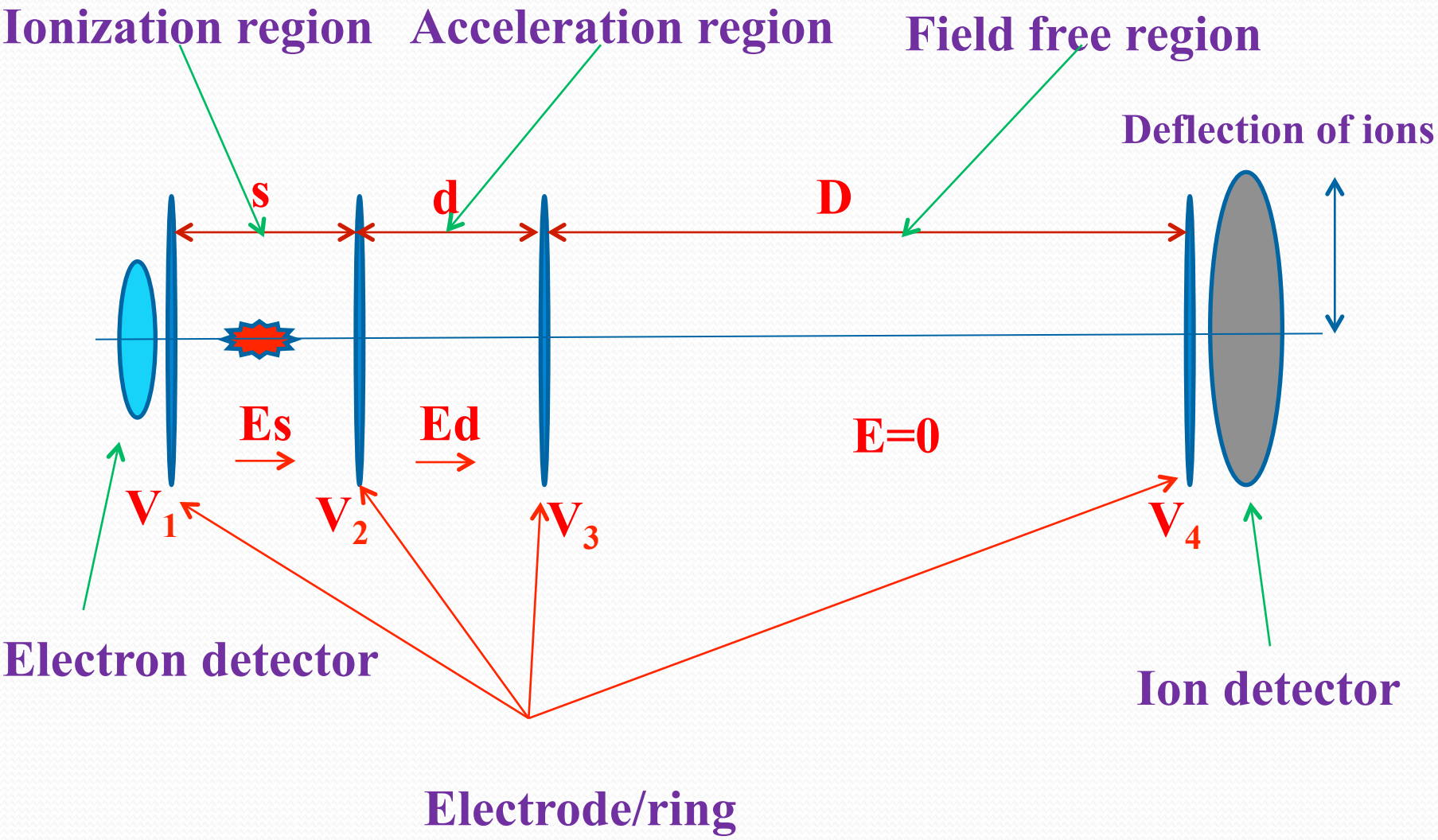
Time of flight mass spectrometer

- **TOFMS is a powerful methodology for the study of the basic mechanisms of ionization of atom and fragmentation of molecules.**

- **TOF with a position sensitive detector , enable us to give kinematically complete analysis of the dissociation process.**

- **TOF spectrometer is used to analyzed positive or negative ions according to their mass to charge ratio.**

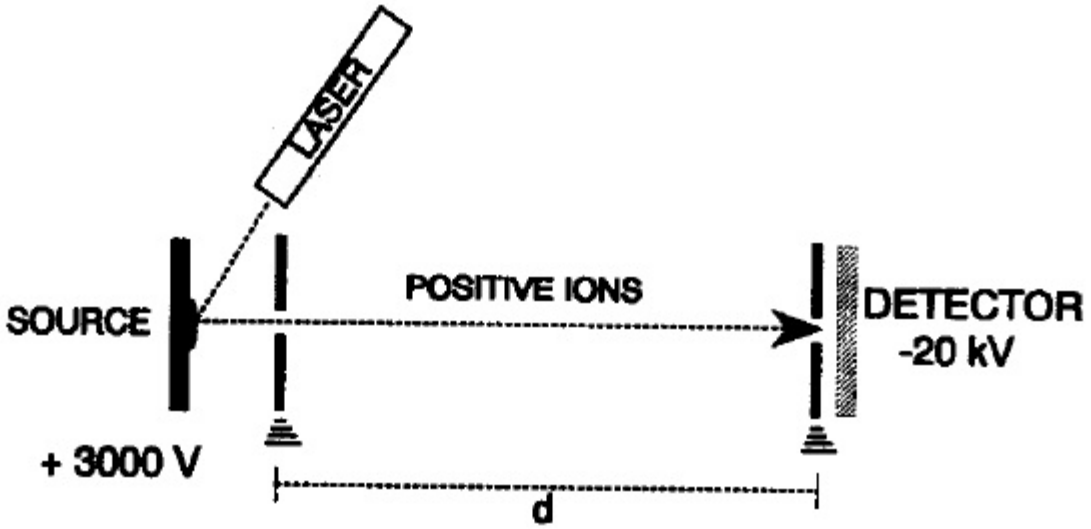
Basic geometry of the TOF mass spectrometer



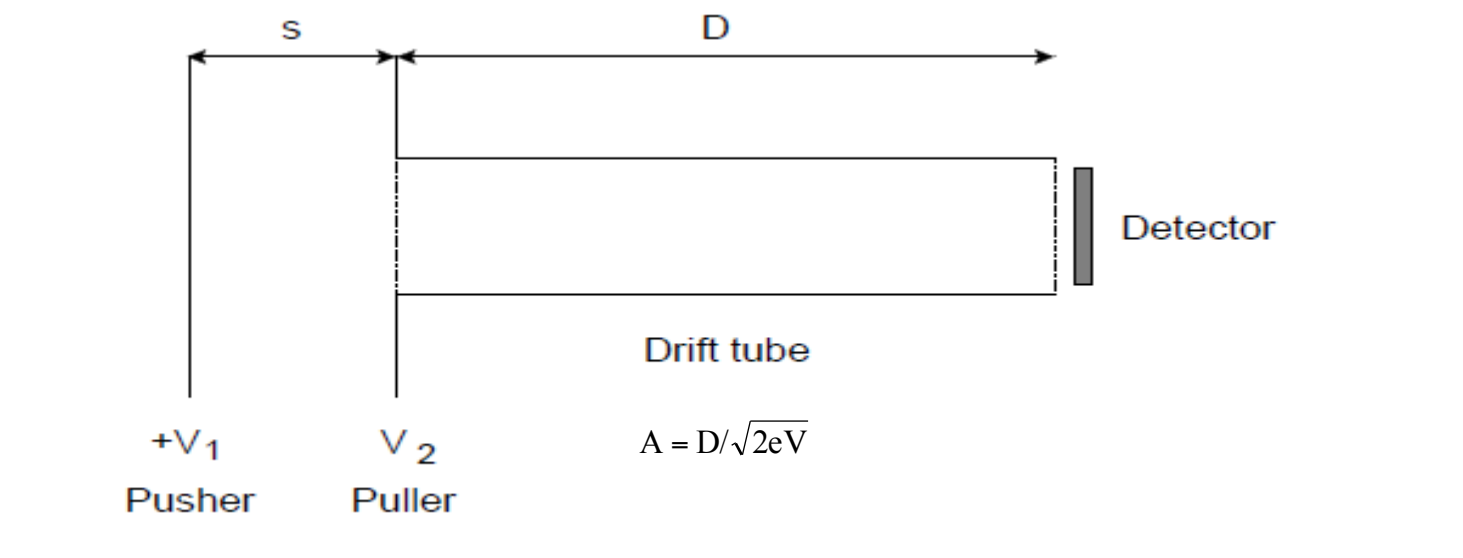
Principle of Time of Flight

Source : ion $\longrightarrow$ $E_{kin} = \frac{1}{2}mv^2 = zV$ $\longrightarrow$ flight tube : d

$$t = \frac{d}{v} \longrightarrow t^2 = \frac{m}{z} \cdot \frac{d^2}{2V}$$



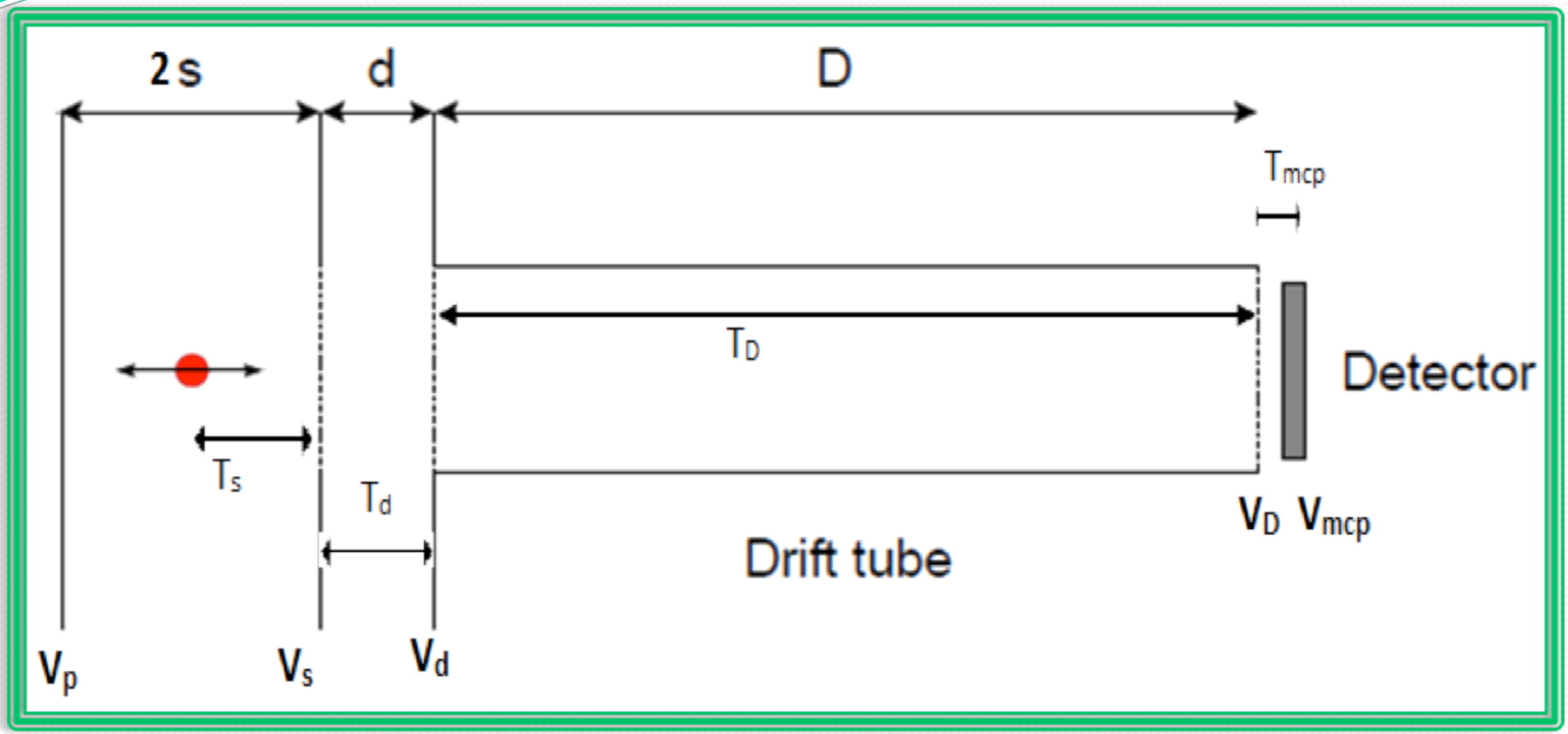
Single Field Time of Flight Mass Spectrometer



$$t = A\sqrt{\frac{m}{q}}$$

Where A is a constant for the given TOF geometry and takes the value, $A = D/\sqrt{2eV}$

Total time for the ion



$$T = Ts + Td + TD + Tmcp$$

where

T s=(vs-us*cos(l))/as

Td=(vd-vs)/ad

TD=D/vd

Tmcp=(vmcp-vd)/a

C- PROGRAMING FOR TOF

```
// m - in kg
// E - in v
//Electric field - in v/m
// Distance - in m
// t-microsecond
//given Energy=5ev,Angle=Varie from 0 to360


#include<stdio.h>
#include<math.h>
#include<stdlib.h>     // Header file for srand and rand functions
#include<time.h>
void newton()
{       FILE *fp1;

     srand(time(NULL));              // Seed for random number generator


    double T1,vs,vd,d,m,vmcp,as,ad,a;
    double D,us,U0,theta,ugiven;
    double q;
    double l,Tmcp,umcp,T0,s,Ts,Td,TD,T,rmcp,Vpos,Vs,Vd,VD,Vmcp;
    double pi;
```

```
int i,iSecret;
pi=3.141593;
rmcp=.015;
s=0.0095;    //half of the distance is considered where interaction happens
d=.114;
D=.247;
Vpos=161.54;
Vs=-161.54;
Vd=-2100;
VD=-2100;
Vmcp=-2150;
m=(2.0)*1.67*pow(10,-27);                    //for deutron
q=1*1.6*pow(10,-19);
U0=5*1.6*pow(10,-19);       // Energy
//   printf("mass= %E\n",m);

if((fp1=fopen("variationofangle5.dat","w"))==NULL)       // create a file for writting
    {
      printf("\n\n error opening output file \n");
    }
    for(i=0;i<100000;i++)
     {
```

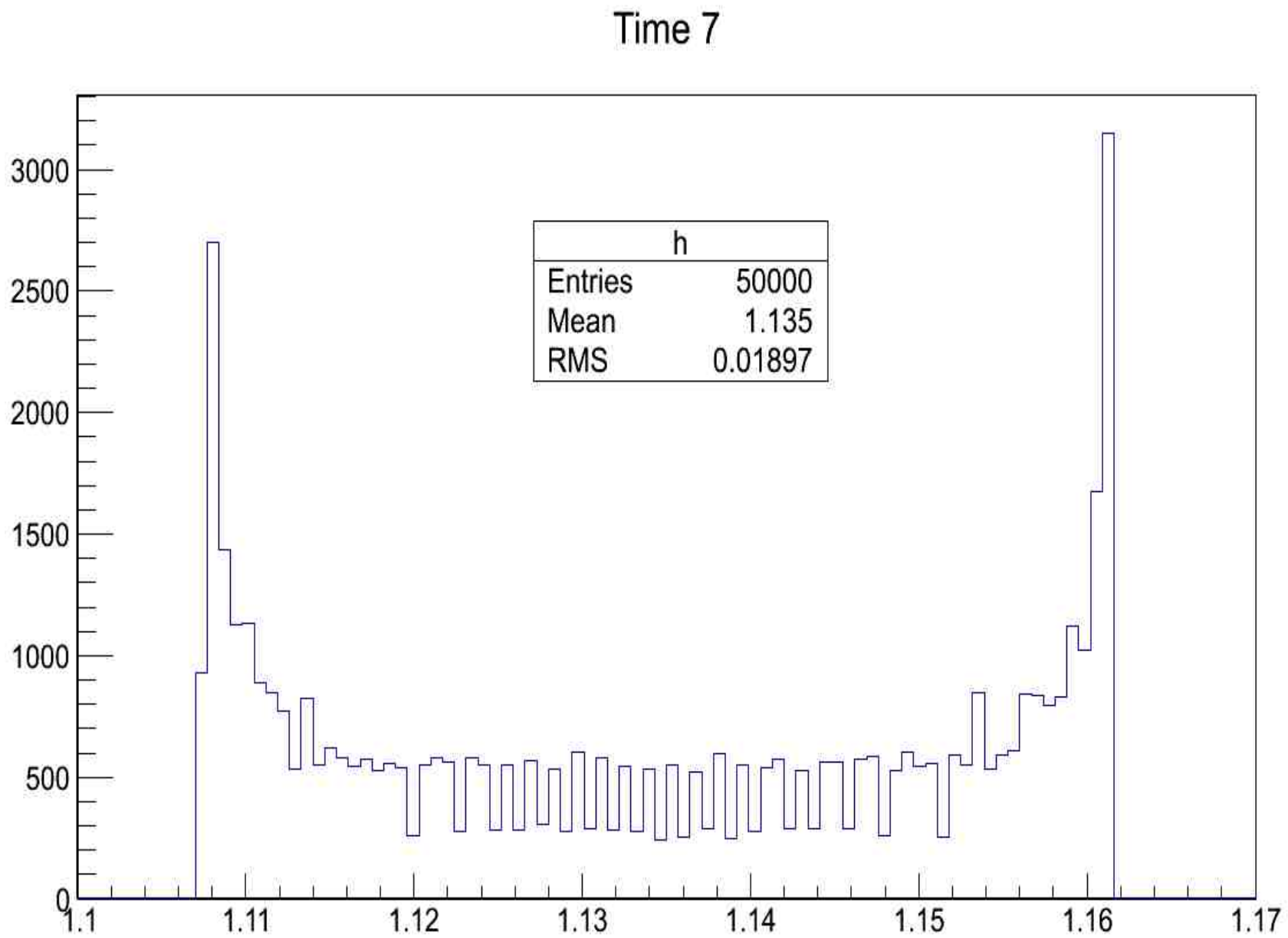
```
iSecret = rand() % 360 + 0;      //   generate random number between 0 to 360
  theta =(float)iSecret;
    printf("theta =%f\n",theta);
l=((theta*pi)/180);
  // (double theta)tion of TOF

          us=sqrt(2*U0)/sqrt(m);                    //initial Velocity
          as=(q*(Vpos-Vs))/(m*2*s);                 //acceleration
          vs=sqrt((us*us*cos(l)*cos(l))+(2*as*s)); // Final Velocity in interaction region

                              Ts=(vs-us*cos(l))/as;

          ad=-(q*(Vd-Vs))/(m*d);
          vd=sqrt(vs*vs+2*ad*d);
          Td=(vd-vs)/ad;

          TD=D/vd;

              a=-(q*(Vmcp-VD))/(m*rmcp);
              vmcp=sqrt(vd*vd+2*a*rmcp);
          Tmcp=(vmcp-vd)/a;
```

```
    T=Ts+Td+TD+Tmcp;
     T1=T*pow(10,6);
       fprintf(fp1,"%f %f\n",theta,T1);
     i=i+1;
   }
 fclose(fp1);
  printf("\nOutput stored in variationofangle5.dat\n\n");
   }
 int main()
   {
  newton();
system("PAUSE");
return 0;
}
```

Program For Drawing Histogram

```
{
TH1F *h=new TH1F ("h","Time 7",100,1.1,1.17);



   Float_t n1,n2;
  Int_t i;
   FILE *myfile;

   myfile = fopen("variationofangle5.dat","r");

   while (!feof(myfile))
   {
      fscanf(myfile,"%f %f\n" ,&n1, &n2);

 h->Fill(n2);
   }

   fclose(myfile);
    h->Draw();

}
```

HISTOGRAM


Time 7
h
Entries 50000
Mean 1.135
RMS 0.01897
3000
2500
2000
1500
1000
500
0
1.1
1.11
1.12
1.13
1.14
1.15
1.16
1.17

Advantage of TOFMS

- Speed at which we can obtain a complete spectrum
- Accuracy depends on the electronics rather on mechanical adjustments

Applications

Environmental Chemistry

- Detecting/quantifying pollutants in atmosphere
- Detecting/quantifying pollutants in water… (http://www.trentu.ca/wqc/)
- Analysis of pollutant/heavy metal uptake in plants/fish
- Atmospheric and space science

Security

- Airport security (ion mobility)
- CSI (always using their GC-MS).
- Drug testing
- Preparative MS (^{235}U)

Industrial

- Quality control (food and pharma)
- Oil and gas exploration

Biological Chemistry

- Monitoring breath of sedated patients
- Detection/quantification of metabolites
- Discovery of cancer biomarkers
- Proteomics!
- Drug discovery (high throughput binding studies)
- Supramolecular structure and dynamics of biological macromolecules


Thank You!

What is TOF

- TOF is a mass analyzer
- Separate according to mass to Charge ratio
- Analogous to monochromator (device used to set apart a small section of a spectrum) in an optical spectrometer

Application

- Environmental chemistry
- Security
- Biological science