G777 2009 Monte Carlo Assignment #1 version 9/14/09

Purpose

The goal of this exercise is to get you to "think like an electron".... to start to think about where electrons from the stream of high energy electrons go when they hit the metal or mineral or semi-conductor or glass you are analyzing. Where do the electrons go in the process of generating x-rays? How big of a region do the x-rays come from? What factors govern the size of this "interaction region"? (Think ... spatial resolution). Do all x-rays in your sample come from the same region? Do the backscattered elections come from the same region? What about secondary electrons?

We have been using Monte Carlo (MC) simulations every year in this class. This week we start with a program developed by David Joy. In the following week we will be running "CASINO", which allows more complex geometries as well as more options for materials.

These programs run under the Windows operating system (though you can run on a Mac if you have Virtual PC software, or on the newer Intel machines, with Bootcamp or Parallels).

You can download the software either from the class ftp site, or directly from the websites of the originators (and some is on the cd that comes with the 3rd edition of Goldstein's textbook, which *should* be in the library).

If you can, run these programs on your own computer (if Windows), otherwise there is a Dell Windows machine in Room 306 ("probe3") with the programs, or you may have access to other Windows computers where you can download the software.

Getting the Software

Getting the software: there are several ways but I suggest the easiest is to bring a memory stick into the probe lab, plug it into Dell Probe3 computer (on floor near AC unit) and copy all 4 programs in the 777 Probe Class folder on the desktop (Casino, GMRFilm, MonteCarlo-Mcfor VB, WinXray). You could also download off the class web page, or go to the author's (in some cases) website.

For the hard core….

You could first read/skim the 1991 Scanning Microscopy paper by Joy (An Introduction to MC Simulations) to get a better general understanding of what these programs are modeling—though it is not necessary.

McforVB, Monte Carlo for Visual Basic, is great for demonstrating most of the points here, but is limited in not allowing any direct input of compositions, rather you have a limited set of mainly pure elements (Cu and 10 metals, plus some tissues) to select from. Next week we will be using a more versatile Monte Carlo program, CASINO, which allows you to enter any material you desire.

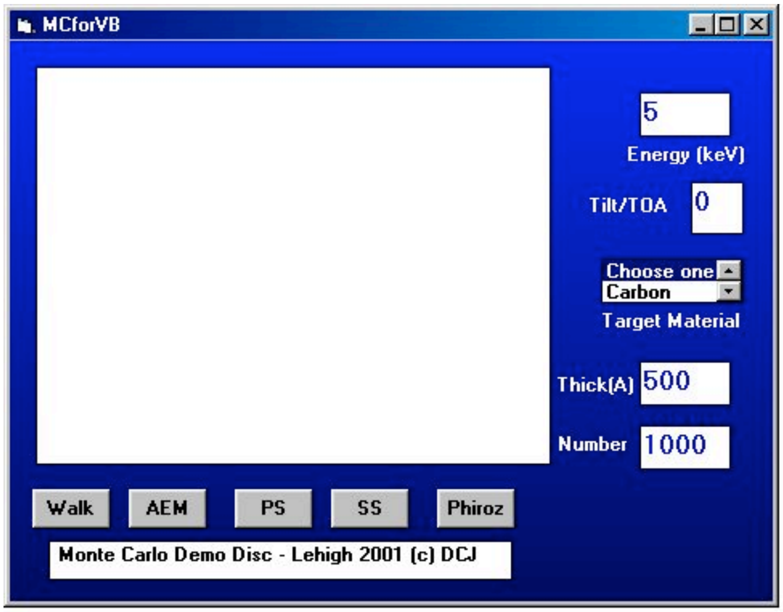
MC_Demo - Monte Carlo Modeling for WIN98

Created by David Joy, modified for G777 UW Madison by John Fournelle 9/10/09

Introduction

The program MC_Demo is a group of simulations illustrating the principles of the Monte Carlo modeling of electron-solid interactions. The programs were written by David Joy and are based on the algorithms described in the book "Monte Carlo Modeling for Electron Microscopy and Microanalysis" published by Oxford University Press (1995). "MC_Demo" is in the public domain and may be freely copied and distributed. If you use results from this package in a publication or presentation an acknowledgement would be appreciated.

This program is designed to run under Window 95 or 98, but works fine under XP. If you downloaded the program be sure that the files MC_Demo.exe and VB40032.dll are placed in the same sub-directory. To run the program choose "Run" from the Start menu and use the "Browse" command to reach the directory where the program is stored. For example, if the program is on a floppy disc, then in the "Run" edit box enter "a:\mc_demo.exe" and then click on "Run". The screen will appear as shown in the illustration. The five programs in the demo are accessed by clicking on either the "Walk", "AEM", "PS",”SS” or "Phiroz" buttons. If you want to print any of the displays simply hit the Print Screen key while holding down the ALT or ALT/SHIFT keys. The screen is then copied to the clipboard. To view, edit, or print these images open the PAINT program - which is usually supplied free as part of the WINDOWS installation in the Accessories file - go to the Edit menu and then click on Paste.



Energy (keV): 5
Tilt/TOA: 0
Target Material: Choose one / Carbon
Thick(A): 500
Number: 1000

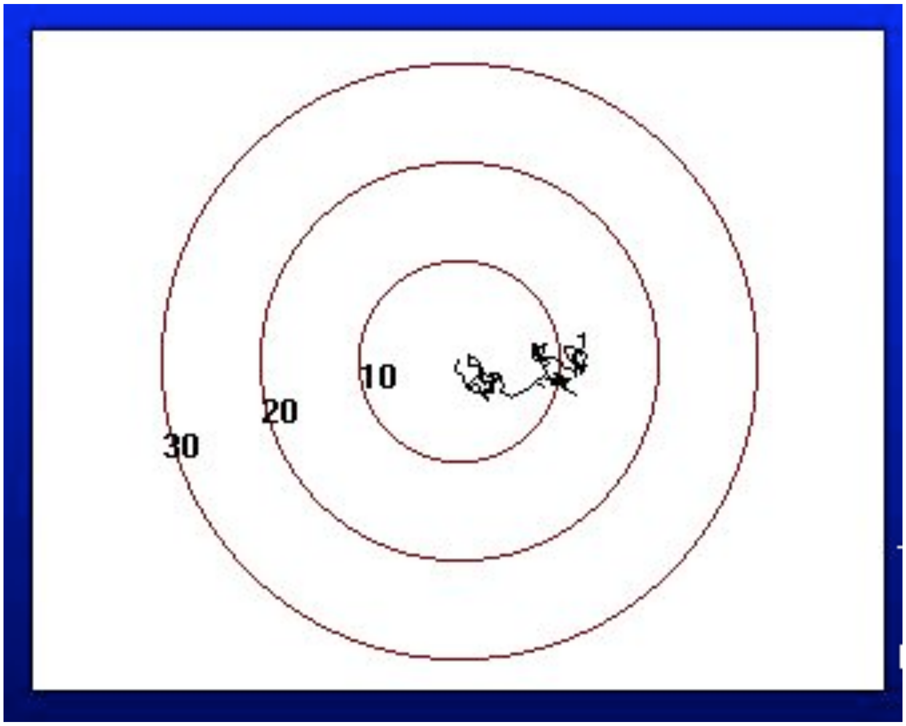
Monte Carlo Demo Disc - Lehigh 2001 (c) DCJ

The program obeys all the usual WIN rules. To change any of the parameters, such as the Energy, click the Mouse in the text box, then either use the delete key to remove the old value, or hold down the left mouse button while dragging across the numbers, and then enter the new value required. NB: In screen shots below, its show SEM1 and SEM2 buttons, instead of PS and SS.

Running the Programs

<u>(1) WALK</u>

This program has nothing to do directly with electron interactions but it is a Monte Carlo simulation and it illustrates some of the concepts of using this technique. It seeks to answers the question - how far away from your starting point would you be after taking N steps each of equal



length in random directions. To run WALK firstly choose the number of steps that you wish to model by entering the appropriate value in the "NUMBER" window . Then click on the WALK button. you can decide how many steps to take. The program then starts and the display shown here appears on the screen. The display shows the progress of the walker and circles representing 10, 20 and 30 steps from the origin are placed on the screen to give an idea of the scale. At the end of the walk the actual distance from start to finish is computed and displayed in the information box immediately underneath the display window.

Experiments and questions:

(a) select a journey of 100 steps and run the program as described above. Note down the reported value of the distance traveled. Now repeat this operation ten times.
Write down your values
How do the values compare ? Why are they not all the same ?

In measuring x-rays, we use something called “1 sigma” as a measure of assumed randomness in any measurement of a “population”. Take 2000 xray counts. One sigma is the square root of 2000, or 44.7 (round to 45). This means that if you take the measurement of the same sample under the exact same conditions, you would say that any measurement between 1955 and 2045 is “statistically the same as any other measurement within one sigma” or that you can assume a population of said measurements will have some randomness, but that it is all still the same thing. If we get more precise in our terminology (and look in a statistics book), we learn about “the normal distribution” within a population and that you can expect 67.4% of a population to be within one sigma of the “true value”, 95.4% within 2 sigma and 99.7 within 3 sigma. We can also speak of this one sigma as a “counting error” type of “standard deviation”.

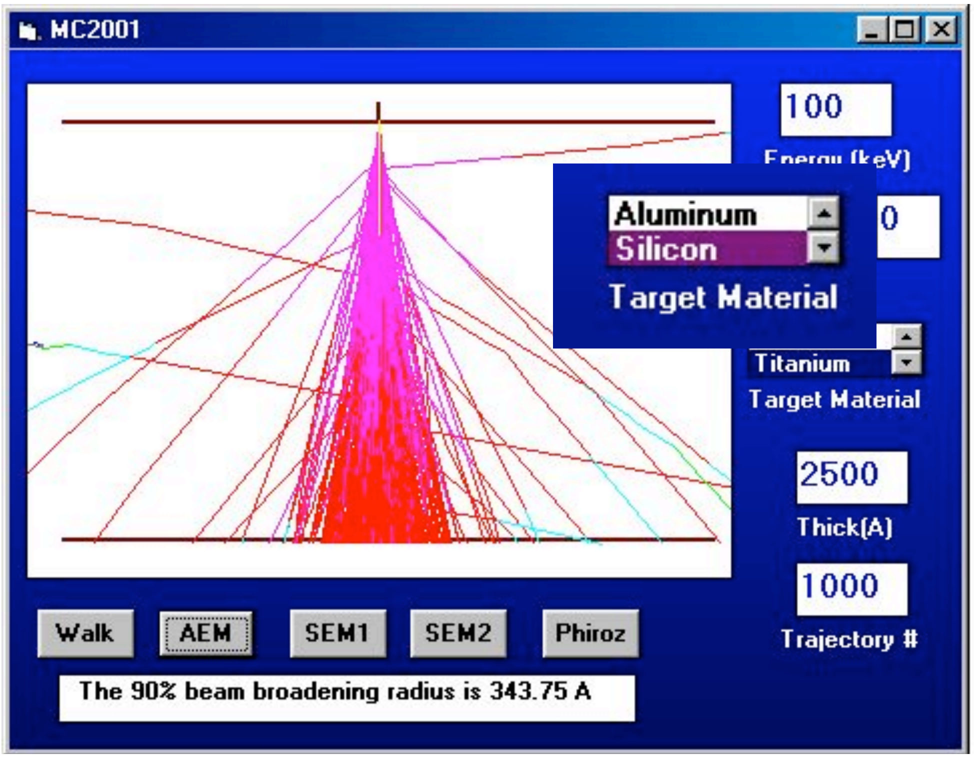
(b) Now repeat these operations (10 of each) for 500 and 5000 steps. Plot the distances for each trial and number of steps on the same graph. Does the distance traveled in a single trial vary in a simple manner with the number of steps ? Why not ?

(c) How does the average distance traveled in N steps (i.e the mean value derived from the ten tries) vary with N ?

You should be able to show from your data gathered in these experiments that the average distance traveled in N steps is equal to the square root of N. In order to demonstrate this however we must perform enough trials at each number of steps to get a statistically valid answer. A single run of the program is not sufficient to provide meaningful results. If you keep the same number of steps and simply re-run the program M times then the variance of the result will be equal to the square root of M. So if you run the program 4 times with the same conditions the expected precision of the average distance calculated is only 50%. If the same conditions are used for a hundred simulations then the precision of the average distance traveled will improve to 10%, and so on.

Important: The point of this exercise is NOT to simulate electrons in solids – rather to show how for random processes [x-ray generation], you need good statistics (large numbers!) to be able to see trends that are real, through the "noise" of randomness.

<u>(2) AEM</u>



100 Energy (keV)

Aluminum
Silicon
Target Material

Titanium
Target Material

2500 Thick(A)

1000 Trajectory #

The 90% beam broadening radius is 343.75 A

SS_MC is a **s**ingle **s**cattering Monte Carlo electron simulation for thin foils. This is, within the overall limits of the approximations used, the most accurate model available. The program is designed for a thin sample – like in the TEM. Start by selecting a beam energy in the "Energy (keV)" box. 100keV is a good value. To select a sample material use the scroll box marked "Target Material" and click the up or down arrows to reach the specimen of choice. Then click on that material and it will be highlighted as shown above. Select a thickness for your sample in the box marked "Thickness (A)" - 1000 (angstroms) would be a good choice. Finally choose how many trajectories you wish to run by editing the contents of the "Number" box. Remembering the previous experiment, the larger the number that you choose the more precise the result will be. A suitable minimum value would be 1000. When you have set up the values you want click on the "AEM" button and the program will run with the display shown. The foil is shown as a cross-section with the beam entering from the top and exiting through the bottom. The thickness of foil that you selected calibrates the scale of this figure. The electron trajectories are color coded to demonstrate any loss of energy that occurs. The information box below the display window computes the beam broadening radius - which is the radius within which 90% of the transmitted electrons lie as the exit from the sample. This effectively defines the expected spatial resolution of an X-ray analysis in this sample.

Run these simulations:

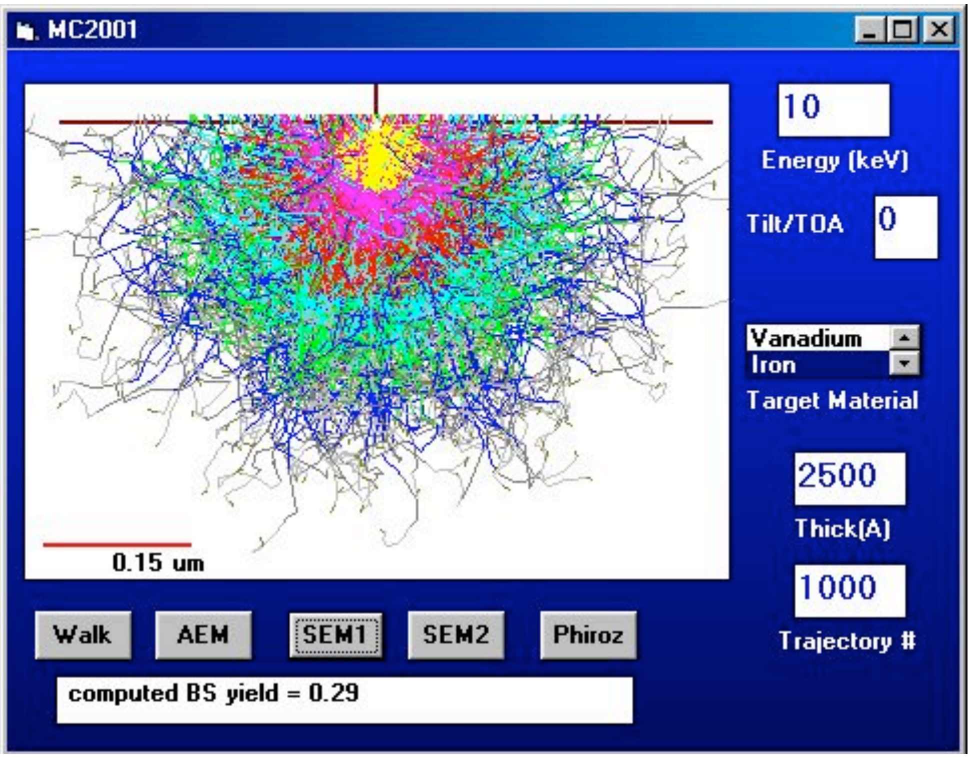
(a) Using copper as the material, observe the beam broadening for an incident energy of 100keV and for sample thicknesses of 250, 750, 1500 and 2000 angstroms using 1000 trajectories per run. How does the broadening vary with the foil thickness? What happens if the beam energy is increased to 200keV?

(b) Repeat experiment (a) but for foils of carbon and gold. What is the effect of making the foil of an element of higher or lower atomic number ?

(c) Using 1000 angstroms of copper as the target observe the trajectories as the incident energy is changed from 100keV to 30, 15, 10, and 5 keV. Notice that "thin" foil starts to behave like a bulk specimen as each electron is scattered many times ?. Note that at low energies each trajectory may take a considerable time so select only 500 or 1000 trajectories and be patient.

There are two observations you need to look for as you change (1) E0 and (2) material composition (atomic number, Z): how the scattering changes and how the incident electrons lose energy, shown in the progression from yellow to purple to red to green to blue to gray.

(3) PS



Energy (keV) 10

Tilt/TOA 0

Target Material: Vanadium
Iron

Thick(A) 2500

Trajectory # 1000

computed BS yield = 0.29

PS is a plural scattering Monte Carlo model which is well suited for studies of electron interactions in bulk specimens (that is, specimens which are not thin enough to transmit the electron beam) and at low beam energies (<20keV). It is slightly less accurate than the single scattering model (SS) but much faster. Start by selecting a beam energy, a material, an angle of incidence (0 means the beam hits the surface at 90 degrees) and the number of trajectories required. The "Thickness" value is not used in this module and so this number has no effect. When everything is set up click on the

"PS" button and the program will start to run. The display carries a calibrated micron marker to aid interpretation of the computed interaction volume. The electron trajectories are color coded to show how the electron loses it energy as it travels. When the chosen number of trajectories has been completed the information window displays the calculated backscattering coefficient ("BS yield").

These "pictures" are a good graphical way to see the extend of electron scattering. The average total distance that the electrons travel is called the "electron range". Interestingly, if an electron reverses path, the range still is the total distance traveled, not the maximum distance from the point of impact.

For the table below, compute the interaction volume depth-radius as NOT the maximum extent of electron travel, but as the limit to about 90% of the electrons, which is what produces virtually all of the signal.

Run these simulations with 5000 trajectories and run 3 experiments at each condition. Note that this is for BULK specimens.

(a) Using 15keV, run 4 different materials: C, Si, Cu and Au. Fill in the table attached at last page, with the electron ranges—E ranges-- (in microns) and BSE coefficients (expressed as fractions). .
(b) Repeat the 4 materials at 30 keV.
(c) Repeat the 4 materials at 5 keV.
These extremes – in E0 and in Z (atomic number) help show basic trends that you need to understand.

Write a summary paragraph. Discuss the effect of E0 on the amount of electron scattering/interaction volume. Discuss the effect of Z. Discuss how BSE coefficient changes (at constant E0) in materials of different Z. Is there much difference in the BSE coefficient in any one material as E0 is changed?

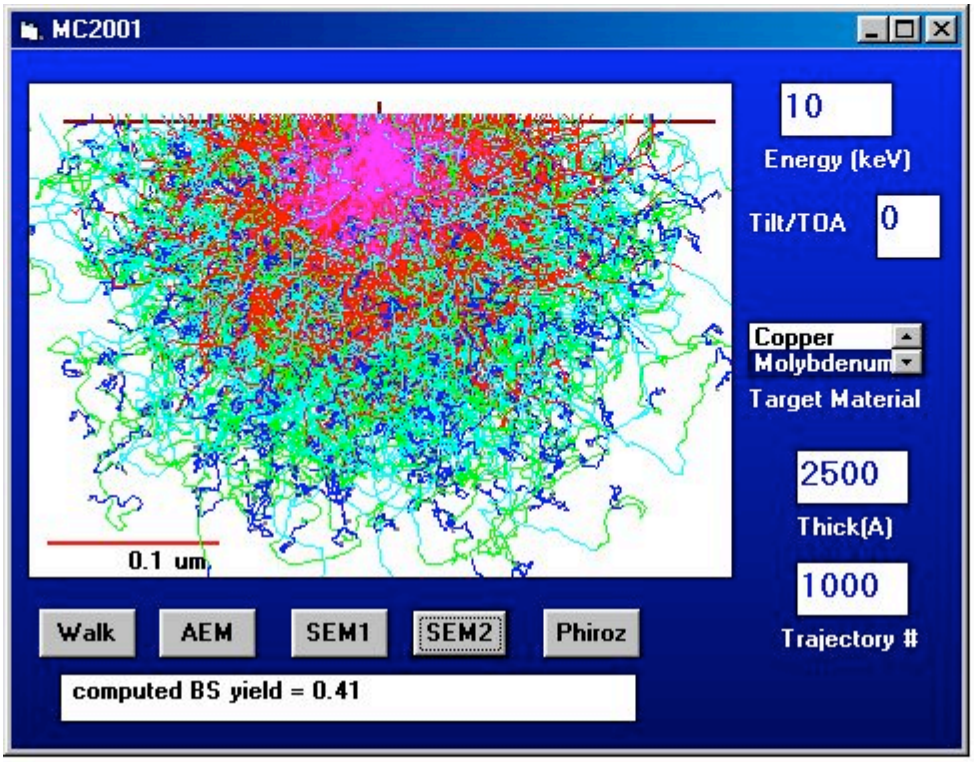
		15 kV	30 kV	5 kV	15 kV	30 kV	5 kV
Element	Z	E range	E range	E range	BSEcoef	BSEcoef	BSEcoef
Carbon							
Silicon							
Copper							
Gold							

========================G777 ___END========================

(There are two other simulations below included here that I will not be assigning you to run. But you are welcome to play with them if you are curious…)

4) SS

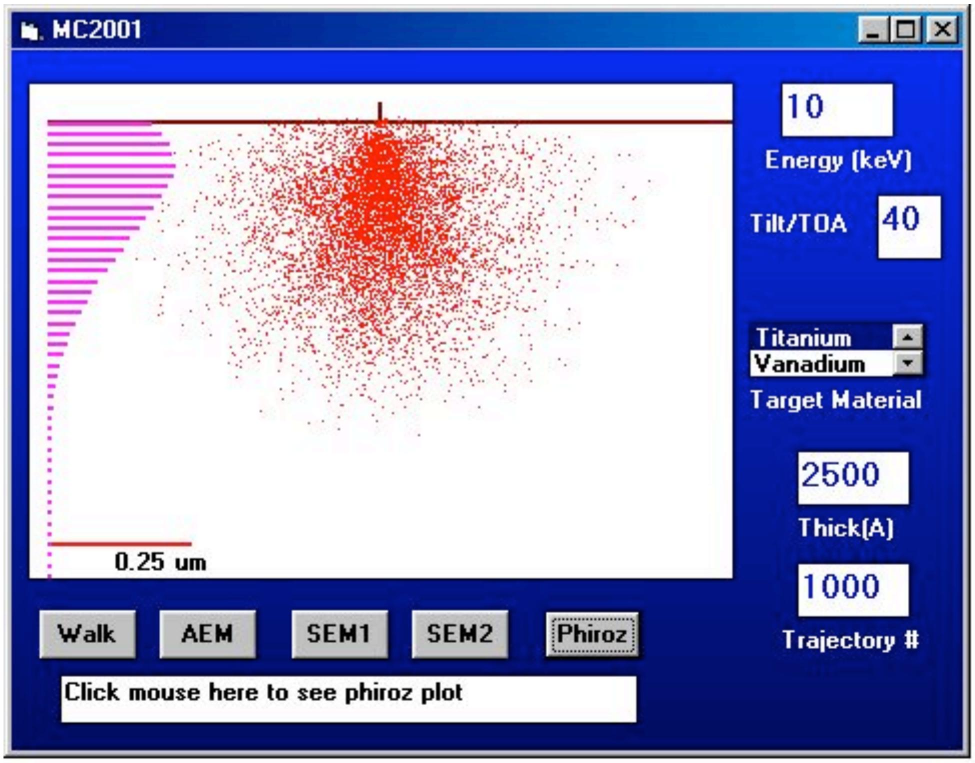
SS is another example of the single scattering algorithm here given in a version designed for bulk samples only. Once again the relative energy of the beam is shown on an arbitrary color scale. The operation of this program is that same as that for PS, but the routines run more slowly because significantly more calculations are involved. To compare this option with SEM1 re-run the trial applications suggested above.



Energy (keV): 10
Tilt/TOA: 0
Target Material: Copper
Thick(A): 2500
Trajectory #: 1000
computed BS yield = 0.41

PHIROZ

This program computes the way in which the yield of a given X-ray line varies with vertical position from the surface. This is called the $\phi(\rho z)$ ("phi ro zee") profile. If this yield is normalized by the equivalent yield for the same X-ray from an infinitely thin region at the surface of the specimen then the resultant ratio is called $f(\chi)$ ("f chi"). This quantity is of fundamental importance in the development of methods for the quantification of X-ray data from solid specimens. To run the program, select an energy, material, and number of trajectories as before. In addition the “Tilt’TOA” box allows selection of the X-ray take off angle into the detector. If no value if given then a default value of 40 degrees is assumed. Provided that the material selected has an X-ray of suitable energy to be excited then the program will run. then click on "PHIROZ". The program displays a simulation of the production of X-rays using a routine originally devised by Curgenven and Duncumb in their classic paper. The density of dots gives an indication of the local rate of X-ray production but is not necessarily directly proportional to the X-ray yield. Note that the X-ray production varies considerably both laterally and in depth. When the run is finished the histogram is plotted on the left hand side of the screen starting at the surface. The length of the bars shows the relative of value of $\phi(\rho z)$ at that depth. The bar at the surface is of unit value. This histogram is plotted at vertical increments equal to 1/50th of the Bethe range. Use at least 500 trajectories to give reasonable statistics.



10
Energy (keV)

Tilt/TOA 40

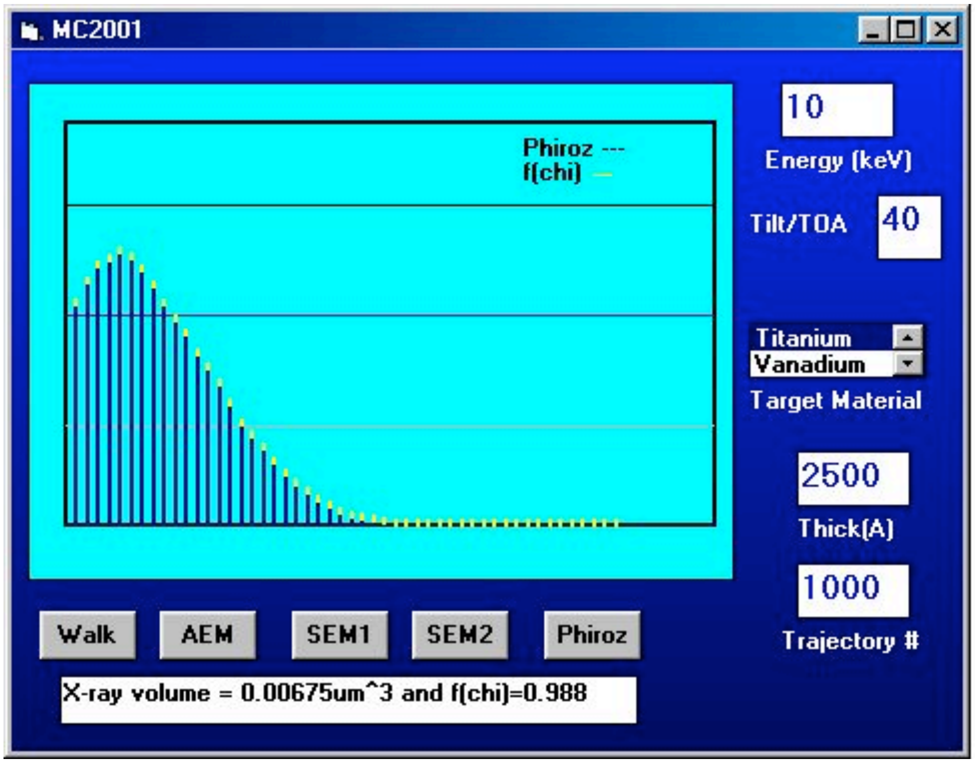
Titanium
Vanadium
Target Material

2500
Thick(A)

1000
Trajectory #

Click mouse here to see phiroz plot

When the program has finished click the mouse inside the information box. The screen will now redisplay the $\phi(\rho z)$ histogram, on a properly annotated scale, together with the corresponding $f(\chi)$ histogram. $f(\chi)$ shows what fraction of the generated X-ray production actually escapes from the specimen after allowing for absorption in the specimen using the take-off angle selected during the set-up. Note that at low voltages the two histograms are very similar, but when the beam energy is much higher than the excitation energy the $f(\chi)$ curve falls away because of strong absorption for X-rays coming from deep into the sample. The information box reports the numerical value of $f(\chi)$ as well as the volume (in cubic micrometers) from which 90% of the total emitted X-ray signal is generated.



Energy (keV): 10

Tilt/TOA: 40

Target Material: Vanadium

Thick(A): 2500

Trajectory #: 1000

X-ray volume = 0.00675um^3 and f(chi)=0.988

Suggested trial applications:

(a) for copper at 20keV obtain the $\phi(\rho z)$ curve . Now repeat the experiment for an incident energy of 10keV. How do the two curves compare? Why is there a difference?

(b) Compute the $\phi(\rho z)$ curve for carbon at 3, 10, and 20keV. Compare the $\phi(\rho z)$ curves at these energies, as well as the $f(\chi)$ value. Why does $f(\chi)$ decrease as the beam energy is increased?