X-RAY ATTENUATION CORRECTIONS FOR HUMAN HEAD HAIR USING PIXE

by

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of a senior thesis submitted by

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This thesis has been reviewed by the research advisor, research coordinator, and department chair and has been found to be satisfactory.

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ABSTRACT

X-RAY ATTENUATION CORRECTIONS FOR HUMAN HEAD HAIR USING PIXE

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This thesis paper examines the feasibility of using correction factors on human head hair with PIXE spectroscopy. Using computer models, we compared x-ray production from thin samples made by a lengthy acid-digestion process and thick samples which require minimal preparation. By comparing the two numbers, we determined experimental correction factors for hair in thick targets.

This paper first describes the properties of hair and how PIXE is used in trace element analysis. It then details the separate computer programs used to collect data. The resulting x-ray counts are shown with an analysis on how the data are used to determine the corrections.

We found that the computer programs are an accurate representation of the hair for proton energy loss. We determined correction factors, but were not able to experimentally test them due to time and equipment constraints.

ACKNOWLEDGMENTS

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Chapter 1

Introduction

1.1 Overview

Hair is a unique biological material which grows at a steady rate for long time periods. Because it is metabolically inert and contains relatively large amounts of heavy metals, trace-element analysis of human head hair has been widely studied to find relationships between such things as trace elements and disease, occupational hazards, and archeological investigations [1]. A popular technique for trace element analysis of hair is Particle-Induced X-ray Emission (PIXE) spectroscopy because of the high level of precision with which trace elements can be measured. The particles are usually high-energy protons that are directed toward a target and strip electrons from inner-shell orbits in the target atoms. These vacancies in the inner shells are filled by electrons from higher shells, giving off excess energy in the form of x rays. Since each atom has a unique ionization energy, the x rays have a unique spectrum. A heavy concentration of an element will produce a peak in the x-ray emissions from the sample which will identify the element. For elements with atomic number Z less than 60 the K x rays (shell $n=1$) are seen in the spectrum. For higher Z, the L x

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rays (n=2) must be used. Depending on the transition, x rays with slightly different energies can be detected, predominantly the Kα (n=2 to n=1) and Kβ (n=3,4,5... to n=1) x rays.

Hair sample preparation normally requires a lengthy cleansing and acid digestion process in order to make a PIXE target that is less than 5 μm in depth [2]. This process destroys the original hair and, depending on the cleansing method, can remove trace elements [3,4]. Thicker targets can be used, but corrections for x-ray attenuation must be obtained.

1.2   Physical and Chemical Properties of Human Hair

All hair consists of a thin outer cuticle layer with the majority of the hair consisting of the cortex. Because of its thin size and similar composition, the cuticle is considered to be the part of the cortex. Human head hair is unique in that it usually also contains a central core called the medulla. The medulla is usually ignored in scientific research because it "contribute[s] negligibly to the chemical and mechanical properties of human hair fibers" [5]. Chemically, hair has a fairly ordered molecular structure, composed of five main elements: H, C, N, O, and S. The majority of the hair mass is in the form of α keratose and β keratose [6]. Physically, straight hair is cylindrical in nature, with curly hair being more wedged-shape in cross-section. This paper focused on straight hair because of its easy geometry and because my hair is straight.
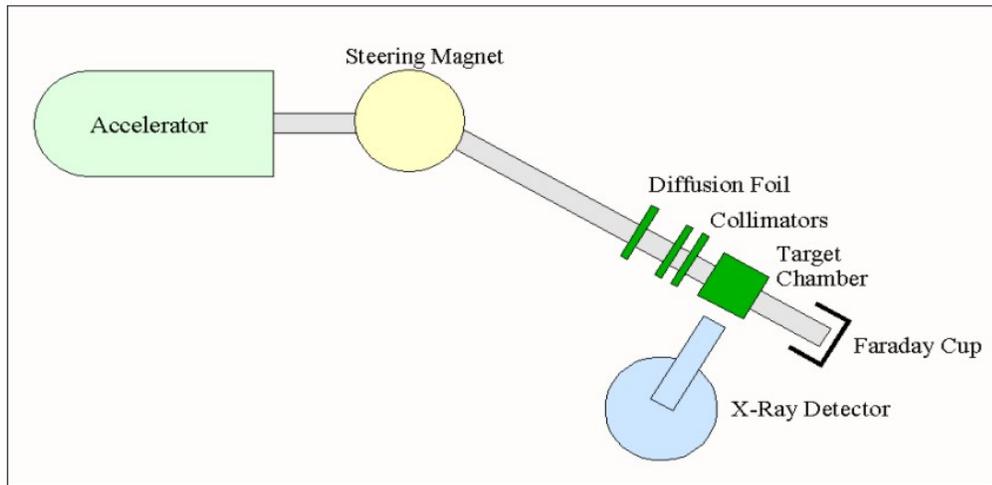
Figure 1.1 PIXE setup

1.3   PIXE

The BYU PIXE group has a 2.17 MeV Van de Graaff proton accelerator. Protons at rest are accelerated by electric fields and pass through a bending magnet. The bending magnet ensures a nearly monoenergetic proton beam since protons with energies greater than or less than 2.17 MeV will smash into the walls of the magnet. The protons travel down an evacuated chamber and are spread out by a diffusion foil which spreads the beam over a larger area of the target. The beam size is adjusted by collimators. The x rays travel to a Si(Li) detector after going through a 14 mm mylar absorber which blocks most of the low-energy x rays. A Faraday cup is connected to a charge integrator which measures the integrated beam current. By knowing how many protons went through the sample, quantitative values for trace elements can be determined. The protons interact with the atoms in the specimen, causing an ionization event which either produces an Auger electron or an x ray. The probability of an ionization event is related to the ionization cross-section of the element. This is
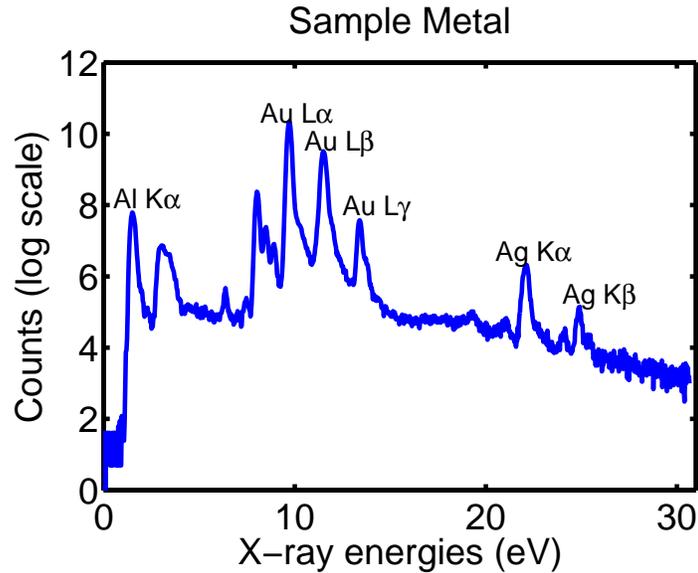
Figure 1.2 Sample spectrum taken from AuCu standard

different from the geometric cross-section of an atom. The interaction cross-section is an area that has the highest probability of causing an event if the proton passes through that area. The cross-section σ is dependent on the energy of the proton beam and atomic number (Z) and is defined as

$$\sigma = \frac{\text{ionizations}}{\frac{(\text{beam particles}) \ (\text{target atoms})}{\text{area}}} \tag{1.1}$$

From standard charts, the probability of an ionization event producing an x ray can be determined as well as the probability of producing either a Kα or Kβ x ray.

The x ray counts from the detector are sent to a software program called GUPIX which analyzes the data and displays it in user-friendly graphs (see Fig. 1.2 for an example). Any correction factors that the user needs to input into the calculations are entered into GUPIX which does all the necessary computations. Correction factors are necessary since accurate x-ray counts are needed for quantitative trace-element results.

1.4   Thin vs. Thick Target

The goal of using acid digestion to prepare hair samples is that the thickness of the sample on the slide is small. A target can be considered thin if it has two characteristics: there is no proton energy loss (the energy of the protons leaving the target are nearly the same as the energy of the protons entering the target) and there is no x-ray attenuation (no x rays passing through the target are absorbed before hitting the detector).

Thick targets are specimens with a noticeable decrease in proton energy as the proton beam travels through the specimen. Energy loss must be calculated as the beam penetrates deeper into the specimen since the probability of an ionization event is dependent on proton energy. X-ray absorption must also be calculated. X rays produced in the center of the hair will interact with electrons as they travel towards the detector. The number of x rays passing through a sample decreases according to the relation

$$N = N_0 e^{-\mu x} \tag{1.2}$$

where N_0 is the number of x rays produced at a certain position in the hair; μ is the attenuation coefficient, an absorption variable dependent on Z and x-ray energy, and x is the distance that the x ray travels through the hair on its way to the detector. A thin vs. thick target correction is made for each element by dividing the number of x rays that reach the detector in a thin target by that of a thick target [7],

$$\text{correction} = \frac{\text{thin-target x rays}}{\text{thick-target x rays}} \tag{1.3}$$

Chapter 2

Details

2.1 Overview

The corrections were calculated by simulating a PIXE experiment in Matlab. The programming was divided among five m-files that oversaw four main jobs: Hair dimensions, x-ray production, x-ray attenuation, and proton energy degradation. A central m-file oversaw the five separate m-files and kept track of the number of x rays counted by the detector.

2.2 Hair Dimensions

Hair that is geometrically straight has a fairly consistent cylindrical shape. The hair coordinate axis was defined as having the long axis of the hair be the z-axis, the proton beam traveled down the y-axis, and the x-axis was in the direction of the detector. The hair was placed so that the proton beam struck the hair in the x-z plane (see Fig. 2.1. Protons approach from the left heading in the positive y-axis, and x rays travel toward the bottom of the page toward the detector. The positive z-axis is
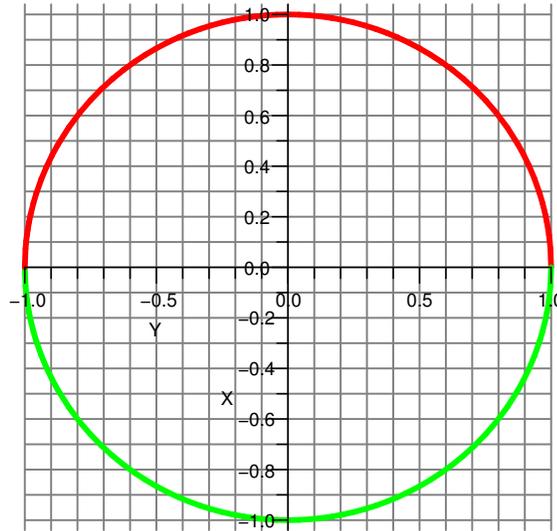
Figure 2.1 Example of a hair being divided into squares in the *x-y* plane.

coming out of the page). The hair was divided up into square areas in the *x-y* plane
with a step size N defined by the user. The hair dimension in the *z*-direction was
fixed at 1 μm. The distance from any square to the bottom edge of the hair where
the detector was located was calculated giving the distance x needed for the x-ray
attenuation calculations. The hair diameter (in microns) must already be known.
This could most easily be determined by optical microscopy.

One major aspect of dividing the hair into square sections was how to deal with
the hair's circular edge. Each square that was on the edge of the hair was run through
a separate m-file that randomly picked a point inside of the square. If the point was
inside the hair, then the entire square was considered hair. If the point was outside the
hair, the entire square was considered vacuum (see Fig. 2.2 for an example of a square
with a random dot that is outside the circle. In this case the entire square would be
considered vacuum). This randomization avoids any bias for too much or too little
hair being represented than is actually present. Running the slice program alone with
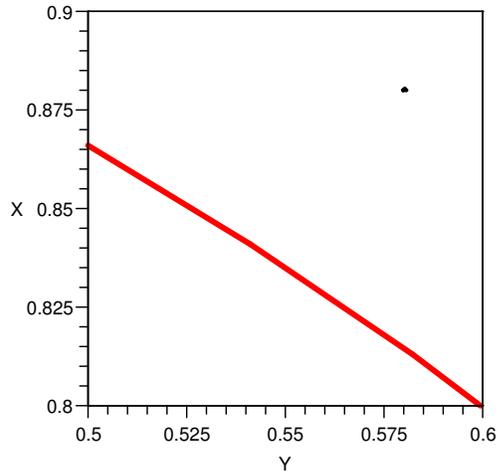
Figure 2.2 Example of a random dot being placed outside the hair

N=700 gives an average error between the cross-sectional area of the real, circular hair and the computerized square hair of .1426 percent with a standard deviation of .0026.

2.3   X-ray production

The first part of x-ray production is the number of ionization events that occur in each cross-sectional area of hair in the x-z plane. The number of ionizations is dependent upon the cross-section (σ) of the atom, which is dependent on Z and the proton energy. Data were obtained for several different σ's for different elements at energies of 500 keV, 1000 keV, 1500 keV, 2000 keV, 2500 keV, and 3000 keV [1]. Using Matlab's interp1 function with the 'cubic' technique and assuming that at 0 keV σ_Z is zero for each Z, σ_Z was found for proton energies to the nearest keV. The number

of ionizations was found using

$$Ionizations = p_0 \rho \delta_y 10^4 N_A \sigma / m_m \tag{2.1}$$

where p_0 is the number of protons in the beam, ρ is the density of the element in the hair matrix, $\delta_y 10^4$ is the depth of the hair in the y-direction that was defined in the 'Hair Dimensions' m-file with a factor of 10^4 to convert from microns to centimeters, N_A is Avogadro's number, and m_m is the molar mass of the element.

Using coefficients found from experimental data, the number of x rays produced from an ionization event is multiplied by a flourescence yield that determines how many events produce an x ray (as opposed to an Auger electron). A separate coefficient constant from the same experimental data determines if a Kα or Kβ x ray is produced (see Fig. 3.2 for a graphical view of Kβ vs. Kα production) [1]. Separate counts are kept for Kα and Kβ x rays for the rest of the experiment.

2.4   Attenuation

Once the number of x rays produced by a given element at a given location in the hair are known, Eq. (1.2) gives the number of x rays that make it to the detector. The distance x was found in the 'Hair Dimensions' m-file. The factor μ has to be calculated for the five dominate hair elements H, C, N, O, and S. μ is found by

$$\mu = CK\lambda^n \rho \tag{2.2}$$

where C, K, and n are dependent on Z and x-ray energy and $\lambda = 12.3981/E$ where E is the x-ray energy [1]. The main m-file kept a count of the total number of x rays N that made it through the hair to the detector.

2.5 Energy Degradation

After the protons went through one square of hair, their new energy had to be calculated before the ionization calculations could be done for the next square of hair. Every element has its own stopping power, or ability to take energy away from the protons. The stopping power S_z is defined by

$$S_Z = \rho \times \frac{dE}{dx} \tag{2.3}$$

where the derivative dE/dx is the proton energy loss as the protons penetrate deeper into the sample. In order to find the energy loss dE I used a parametrization of the stopping power given by Johansson and Campbell [1]:

$$S_Z = \frac{S_L S_H}{S_L + S_H} \times \frac{602.22}{A_Z} \tag{2.4}$$

where

$$S_L = aE^b + cE^d \tag{2.5}$$

and

$$S_H = \frac{e}{E^f} \times ln(\frac{g}{E} + hE) \tag{2.6}$$

with E being the x-ray energy and a, b, c, d, e, f, g, and h are values that depend on Z. The stopping power for H, C, N, O, and S were calculated. These were found in units of $keV\,cm^2/mg$. The actually energy loss E_{lossZ} due to S_Z was found by

$$E_{lossZ} = \frac{S_Z \rho_Z \delta_y}{10} \tag{2.7}$$

where all the symbols have been previously explained. The factor of 10 puts E_{lossZ} in units of keV. The total energy loss is the sum of the energy loss due to each Z,

$$E_{loss} = E_0 - E_{lossH} - E_{lossC} - E_{lossN} - E_{lossO} - E_{lossS} \tag{2.8}$$
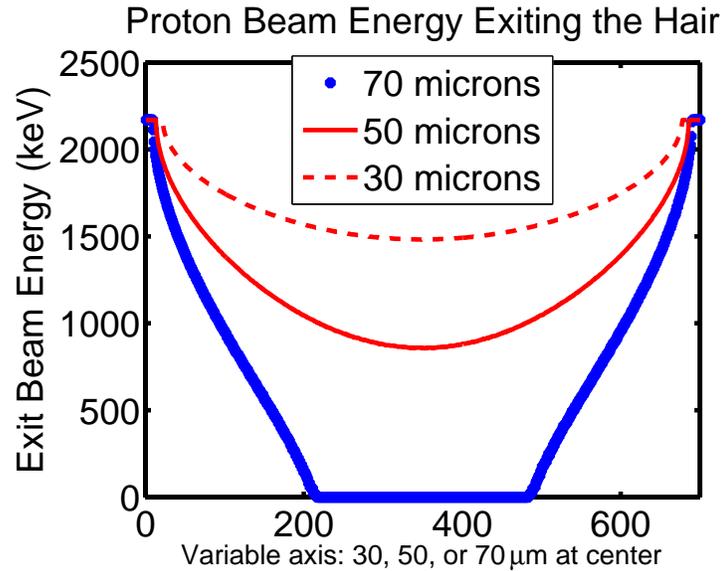
Figure 2.3 Exit-beam Proton Energies

This new energy is returned to the 'x ray' m-file and the whole process is repeated for the next segment of hair with a decreased proton energy. This section of the code was checked against established stopping energies. It was experimentally determined that 2.5 MeV protons have a stopping distance of 55 μm in pure carbon [1]. The 'Energy Degradation' m-file was tested by having 2.5 MeV protons hit a hair that was made of pure carbon. As the step size N increased to 1000, the stopping distance increased to 54.6 μm which is accurate for the two accepted significant digits of 55 μm. Fig. 2.3 shows the proton beam energies as they leave the hair. The x-axis is a variable axis. The two sides of the graph represent a hair thickness of 0 μm that the protons pass through on their way to the Faraday cup, while the middle of the graph represents either 30, 50, or 70 μm of hair thickness. Approximately one-third of the 70 μm hair is thick enough that no protons pass through the hair to the Faraday cup, making what is essentially an infinitely thick target for 2.17 MeV protons. We expect correction factors to be highest for the 70 μm hair for this reason.

2.6 Thin Target

After all of the data are collected for a hair placed in the accelerator, the main m-file takes the same hair and converts it into a thin target. This is done by removing the 'Attenuation' and 'Energy Degradation' portions of the Matlab code and running the file over again. These x rays are then counted and put into separate files from the thick-target files. Graphs are displayed for Kα and Kβ counts.

2.7 Corrections

Initial values for the proton energy (in keV), the number of protons in the beam, the diameter of the hair (in microns), and the step size N need to be input by the user in the main m-file. Because actual experiments will be run on BYU's particle accelerator, the proton energy is 2170 keV. The number of incident protons is arbitrarily set at 10^9. After the program has been run and the total x-ray counts have been graphed for the attenuated and non-attenuated cases, the non-attenuated counts are divided by the attenuated counts to yield the correction factors. These factors are also saved in text files that can be transferred for use on other computers that have GUPIX.

Chapter 3

Results and Conclusion

3.1 K-lines

I ran the programs with a step size $N = 700$ and three different hair diameters of 30, 50, and 70 microns. Fig. 3.1 shows the Kα thin-target x rays for a 50 micron hair. The decrease in counts as Z increases is because the high Z elements have smaller cross-sections than low Z elements for the same proton beam energy. The thin-target Kα x rays are useful for noting that there is an exponential relationship between Z and x-ray count. Fig. 3.2 is a graph of the probability of a Kβ x ray being produced in an ionization event versus a Kα x ray being generated. For Z=11 and Z=12 no Kβ x rays are produced, and there is a low probability of Kβ x rays until about Z=20, and then there is a steady slope until Z=60. This explains the non-exponential fit to Kβ x rays at low Z. The Kβ rays in Fig. 3.1 show that for Z smaller than 20 the Kβ's are not produced as proportional as they are compared to the Kα's at higher Z.

The attenuated x rays are the next results (Fig. 3.3). They had a similar shape as the thin-target Kα x rays, but the counts were less then the thin-target counts
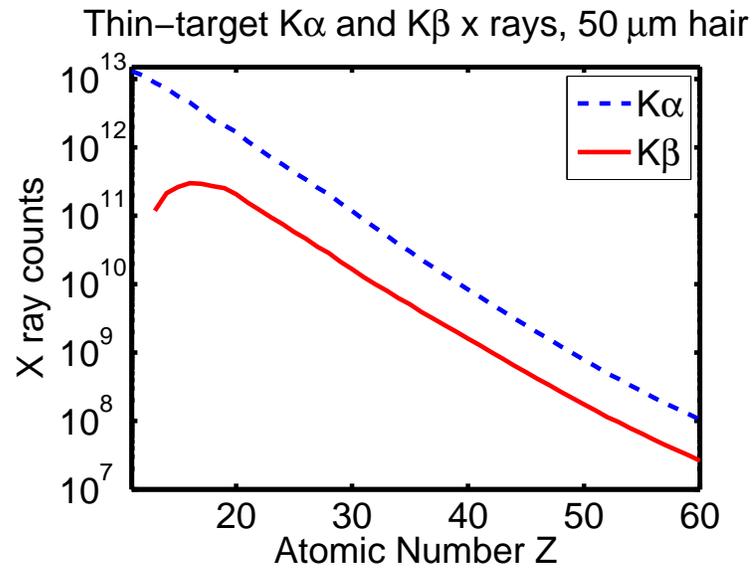
Figure 3.1 Kα and Kβ thin target x-rays.
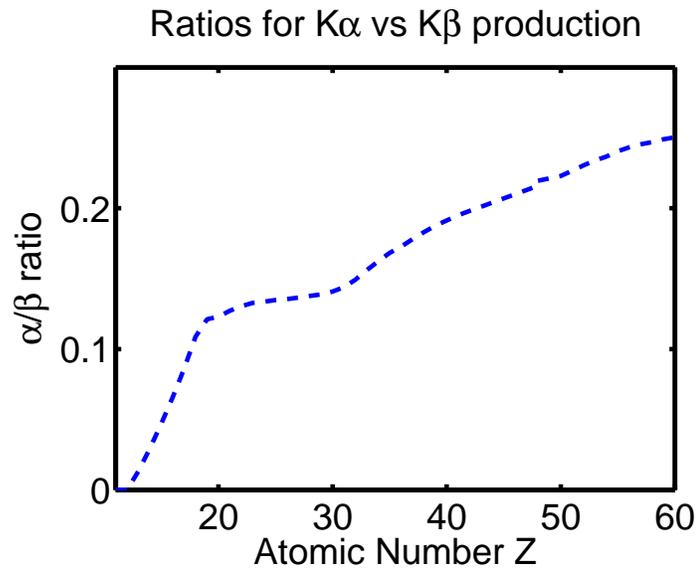
Figure 3.2 Kβ versus Kα x-ray production.
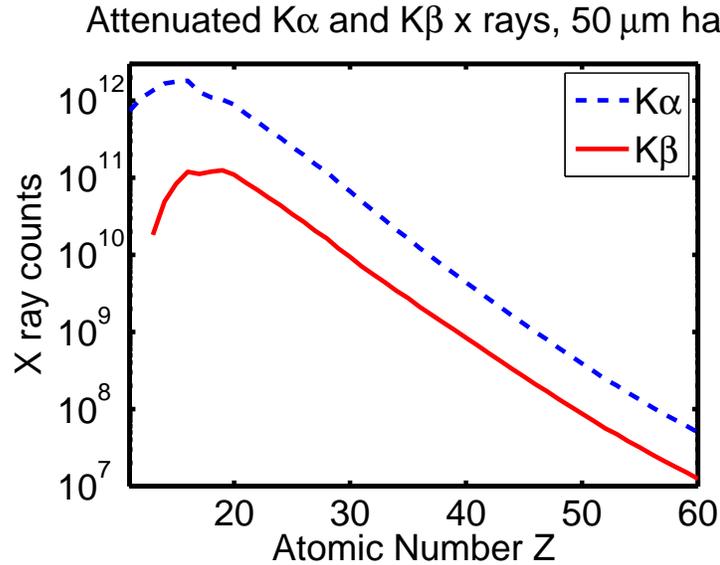
Figure 3.3 Kα and Kβ attenuated x-rays.

for all elements. Both the Kα and Kβ lines peak just below Z=20 and break their smooth curve that they had for higher Z, and then the counts fall off. This is because of the attenuation equation (Eq. (1.2)). The lower the x-ray energy E, the stronger the attenuation. At Z=18 (Ar) the x-ray energy drops below 3 eV, and the x rays are heavily attenuated, so the counts drop off. The Kβ x rays have slightly higher energies than Kα x rays for the same Z but start to be heavily attenuated at nearly the same time as the Kα x rays.

Fig. 3.4 is a plot of the correction value for each element. It is interesting to see that when Kβ's start needing corrections at Z greater than 13 that it is the same correction as the Kα x rays. There is a noticeable bump in the corrections at Z=17 (Cl). Fig. 3.3 shows that around Z=16 that the Kα and Kβ counts are not smooth. The numerical data show that Kα counts peak at Z=16 (S) and do a sudden drop at Z=17, while the Kβ line drops at Z=17 and the counts then continue to increase until Z=19. The peak for S and and the drop for Cl are because of the high amount
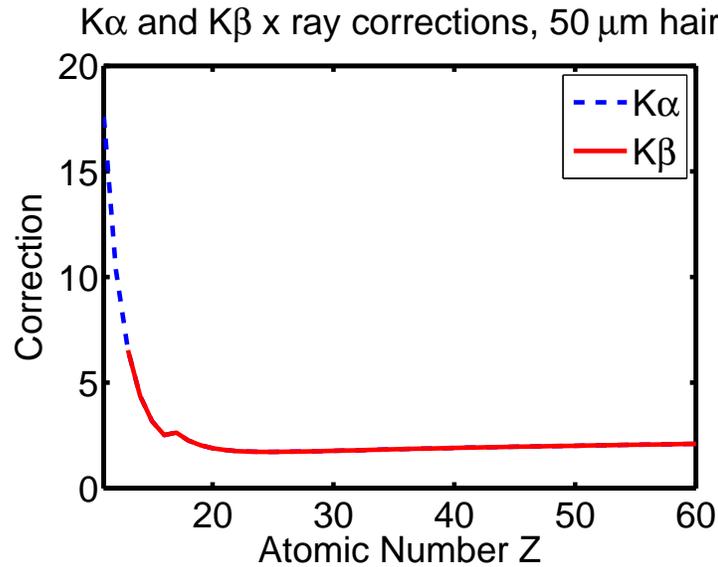
Figure 3.4 Kα and Kβ attenuated x-rays.

of S in human hair. As the x rays travel to the detector they are attenuated by the five main components of hair (H, C, N, O, and S). While the S content in hair varies, there is a commonly accepted average value of about 4.7% that was used in the 'attenuation' m-file. X rays from S atoms are not attenuated by S atoms, so S counts should be higher than the counts for Cl and P (Z=15). However, since Cl x rays have an energy that is slightly higher than the S ionization energy, Cl x rays are absorbed by S atoms and new S x rays are produced. This increases the S count and decreases the Cl count. This is why the correction factor for Cl (Z=17) is higher than the neighboring corrections.

3.2 L-lines

The plot for the Lα attenuated counts shows a similar slope for the three hair diameters (Fig. 3.5). It is interesting to see that the x ray counts are more similar for the 50 and 70 μm hairs than for the 30 and 50 μm hairs. This is because the hair is so
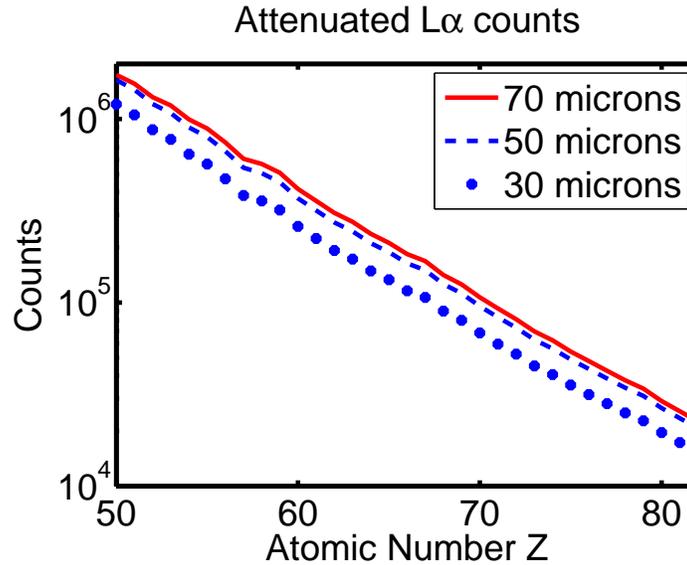
Figure 3.5 Lα attenuated counts

thick that the proton beam is losing all of its energy and is producing a maximum number of x rays. The plot for the Lα thin-target counts shows a slope similar to the attenuated Lα lines, but with higher counts (Fig. 3.6).

The necessary corrections for the Lα lines are shown graphically below (Fig. 3.7). These will be input into GUPIX for real experiments.

3.3   Conclusion

The collected data was compared as best as it could be to experimental values and appears to be accurate. The computed and experimental stopping powers agree very well. The next step of this project would be to prepare thin- and thick-target hair samples for PIXE analysis and determine how well the correction factors agree with experiment.
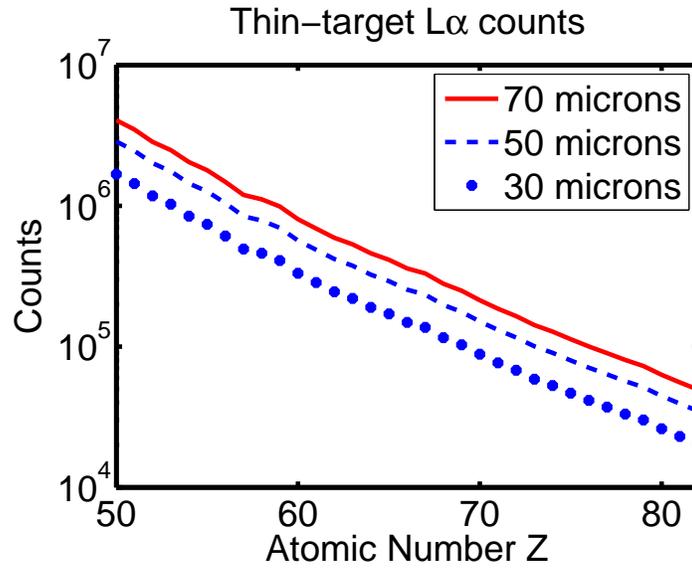
Figure 3.6 Lα thin-target counts
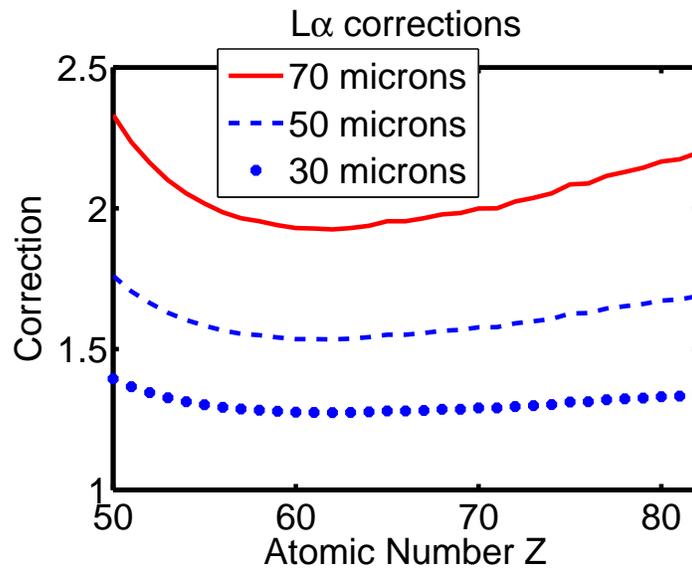
Figure 3.7 Lα corrections

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[7] L. B. Rees, "A Monte Carlo approach to X-ray attenuation corrections for proton-induced X-ray emission from particulate samples," Nuclear Instruments and Methods in Physics Research A **299,** 614–617 (1990).

Appendix A

Matlab Codes

A.1   Main m-file

```
% David Silvers    Start: 14 March 2007
% This is the grandaddy file where everything is controlled.
clear; close all; clc; eq1=cputime;
diameter=50;        % Diameter of the whole hair in microns
N=51;               % Step size
protons=10^9;       % This is the number of protons in the beam.
Ebeam=2170;         % Beam energy in keV
global matrix global matrixbeta global numbers1 global numbersbeta1
global numbers1na global numbersbeta1na global dense global
practice2 global moles global flour1 global powers
numbers1=zeros(50,3); numbersbeta1=zeros(50,3); matrix=zeros(50,3);
matrixbeta=zeros(50,3); numbers1na=zeros(50,3);
numbersbeta1na=zeros(50,3);
load densities2uniform.csv;  % Arbitrary densities of trace elements in hair
```

```
dense=densities2uniform;

load tablea2.csv      % Cross-section data

practice2=tablea2;

load moles.csv        % Molar densities of elements

load tablea1.csv      % Contains fluorescence coefficients and x ray energies

flour1=tablea1;

load TableA8.csv      % Stopping power data

powers=TableA8; counts=zeros(50,3); countsbeta=zeros(50,3);

countsna=zeros(50,3); countsbetana=zeros(50,3);

stopenergy=zeros(N,1); stopenergy(4,1)=12;

% First, give a diameter for the hair and it will return a matrix with the

% hair divided into slices. It also returns the depth of the hair.

[a,delta,b,squarearea,roundarea,error]=slices(diameter,N); for n=1:N

    E=Ebeam;      % Beam energy

    for m=1:N

        if a(n,m)~=0

            %Find the number of ionizations for this nonzero square

            distance=b(n,m)*10^(-4)*delta;  % This is the distance the x-ray must

            [numbers,c,numbersbeta]=xrays(delta,distance,E,protons);

            %Then multiply by the fluorescence yield

            %Then multiply by ratio to find the number of K-alphas and call it N

            %Find distance through hair and find N0=N*exp(-mu*x). Then I need to s

            counts(1:50,1)=numbers(1:50,1);

            counts(1:50,2)=numbers(1:50,2);

            counts(1:50,3)=counts(1:50,3) + numbers(1:50,3);

            countsbeta(1:50,1)=numbersbeta(1:50,1);
```

```
            countsbeta(1:50,2)=numbersbeta(1:50,2);

            countsbeta(1:50,3)=countsbeta(1:50,3) + numbersbeta(1:50,3);

            %Then go to step three.

            % Step Three: Find the energy for the next step and go to the next col

            [E]=stoppower(E,delta);

        end

    end

    stopenergy(n,1)=E;

end countstotal(1:50,1)=counts(1:50,2);

countstotal(51:100,1)=countsbeta(1:50,2);

countstotal(1:50,2)=counts(1:50,3);

countstotal(51:100,2)=countsbeta(1:50,3);

countstotalsorted=sortrows(countstotal,[1]); xdataalpha=counts(:,1);

ydataalpha=counts(:,3); xdatabeta=countsbeta(:,1);

ydatabeta=countsbeta(:,3);

semilogy(xdataalpha,ydataalpha,'r-',xdatabeta,ydatabeta,'b--','LineWidth',2.5)

aa=gca; set(aa,'XLimMode','manual','YLimMode','manual','Xlim',[11

20],'Ylim',[10^3 10^6],'FontSize',20,'LineWidth',2.5) title('K-alpha

and K-beta x-rays, attenuated') xlabel('Atomic Number Z')

ylabel('Counts') figure countsfile=zeros(50,4);

countsfile(:,1)=xdataalpha(:,1); countsfile(:,2)=ydataalpha(:,1);

countsfile(:,3)=ydatabeta(:,1); countsfile(:,4)=ydataalpha(:,1) +

ydatabeta(:,1); placeholder=11:60; xdataalpha1=xdataalpha';

ydataalpha1=ydataalpha'; ydatabeta1=ydatabeta';

countstrial=[xdataalpha1; ydataalpha1; ydatabeta1];

fid=fopen('countstrial.txt','w');
```

```
fprintf(fid,'%12.3f %12.3f %12.3f \r\n',countstrial);

st=fclose(fid);

%Now do the same process for a thin-target

for n=1:N

    E=Ebeam;      % Beam energy

    for m=1:N

        if a(n,m)~=0

            %Find the number of ionizations for this nonzero square

            distance=b(n,m)*10^(-4)*delta;  % This is the distance the x-ray must

            [numbers1na,c,numbersbeta1na]=xraysthin(delta,E,protons);

            countsna(1:50,1)=numbers1na(1:50,1);

            countsna(1:50,2)=numbers1na(1:50,2);

            countsna(1:50,3)=countsna(1:50,3) + numbers1na(1:50,3);

            countsbetana(1:50,1)=numbersbeta1na(1:50,1);

            countsbetana(1:50,2)=numbersbeta1na(1:50,2);

            countsbetana(1:50,3)=countsbetana(1:50,3) + numbersbeta1na(1:50,3);

        end

    end

end countstotalna(1:50,1)=countsna(1:50,2);

countstotalna(51:100,1)=countsbetana(1:50,2);

countstotalna(1:50,2)=countsna(1:50,3);

countstotalna(51:100,2)=countsbetana(1:50,3);

countstotalna=sortrows(countstotalna,[1]);

xdataalphana=countsna(:,1); ydataalphana=countsna(:,3);

xdatabetana=countsbetana(:,1); ydatabetana=countsbetana(:,3);

semilogy(xdataalphana,ydataalphana,'r-',xdatabetana,ydatabetana,'b--','LineWidth',
```

```
aa=gca; set(aa,'XLimMode','manual','YLimMode','manual','Xlim',[11
20],'Ylim',[10^5 10^6],'FontSize',20,'LineWidth',2.5) title('K-alpha
and K-beta x-rays, thin target') xlabel('Atomic Number Z')
ylabel('Counts') figure
%This calculates the corrections
calpha=ydataalphana./ydataalpha; calpha=calpha'; cbeta(1)=0;
cbeta(2)=0; cbeta(3:50)=ydatabetana(3:50)./ydatabeta(3:50);
plot(placeholder,calpha,'r-',placeholder,cbeta,'b--','LineWidth',2.5)
aa=gca; set(aa,'XLimMode','manual','YLimMode','manual','Xlim',[11
60],'Ylim',[0 25],'FontSize',20,'LineWidth',2.5) title('Corrections
for K-alpha and K-beta x-rays') xlabel('Atomic Number Z')
ylabel('Correction Factor') correctionsalpha=[placeholder;calpha];
correctionsbeta=[placeholder;cbeta];
fid=fopen('correctionsa.txt','w');
fprintf(fid,'%12.3f %12.3f \r\n',correctionsalpha);
st=fclose(fid); fid=fopen('correctionsb.txt','w');
fprintf(fid,'%12.3f %12.3f \r\n',correctionsbeta);
st=fclose(fid); fid=fopen('Stopping Energies.txt','w');
fprintf(fid,'%12.3f \r\n',stopenergy);
st=fclose(fid); xdataalphana1=xdataalphana';
ydataalphana1=ydataalphana'; ydatabetana1=ydatabetana';
countstrialthin=[xdataalphana1; ydataalphana1; ydatabetana1];
fid=fopen('countstrialna.txt','w');
fprintf(fid,'%12.3f %12.3f %12.3f \r\n',countstrialthin);
st=fclose(fid); eq2=cputime-eq1
```

A.2   Attenuation

```
% David Silvers    7 March 2007

function [matrix,

matrixbeta]=attenuation(distance,alpharays,betarays,Kalpha,Kbeta,c)

global matrix global matrixbeta

E=Kalpha;       % E is the x-ray energy

rhoHair=1.370; % units of g/cm^3

rhoH=.075*rhoHair; rhoO=.282*rhoHair; rhoN=.136*rhoHair;

rhoC=.46*rhoHair;

rhoS=.04*rhoHair; %.038-.082

                % Hydrogen

                if E>=1 && E<=2

                    muH=rhoH*.0146*(12.3981/E)^3.00344;

                end

                if E>=2 && E<=3.5

                    muH=rhoH*.0589*(12.3981/E)^2.239;

                end

                if E>=3.5 && E<=4.00

                    muH=rhoH*.07434*(12.3981/E)^2.055;

                end

                if E>=4 && E<=6

                    muH=rhoH*.27795*(12.3981/E)^.889;

                end

                if E>=6 && E<=9.2

                    muH=rhoH*.43231*(12.3981/E)^.281;
```

```
end

if E>=9.2 && E<=40

    muH=rhoH*.44767*(12.3981/E)^.1628;

end

muO=rhoO*5.3268*.532*(12.3981/E)^3.041;

if muO/rhoO<1

    if E>=17.2 && E<=25

        muO=rhoO*1.8345*(12.3981/E)^1.8535;

    end

    if E>=25 && E<=40

        muO=rhoO*1.07154*(12.3981/E)^1.08685;

    end

end

muN=rhoN*4.5355*.4016*(12.3981/E)^3.066;

 if muN/rhoN<1

    if E>=15 && E<=21.

        muN=rhoN*1.4641*(12.3981/E)^2.00119;

    end

    if E>=21. && E<=30.

        muN=rhoN*1.06418*(12.3981/E)^1.39578;

    end

    if E>=30. && E<=40

        muN=rhoN*.60023*(12.3981/E)^.74774;

    end

end

muC=rhoC*3.8531*.2838*(12.3981/E)^3.094;
```

```
              if muC/rhoC<1

                  if E>=13 && E<=19.5

                      muC=rhoC*1.10987*(12.3981/E)^2.19895;

                  end

                  if E>=19.5 && E<=27.5

                      muC=rhoC*.74709*(12.3981/E)^1.32494;

                  end

                  if E>=27.5 && E<=40

                      muC=rhoC*.40943*(12.3981/E)^.57;

                  end

              end

              if E>2.472

                  muS=rhoS*10.1931*2.472*(12.3981/E)^2.916;

              else

                  muS=rhoS*1;    % I'm not understanding the chart. Does this

              end

               if muS/rhoS<1

                  if E>=37.5 && E<=40

                      muS=rhoS*6.09135*(12.3981/E)^1.63252;

                  end

              end
alphatotal=alpharays*exp((-muH-muO-muN-muC-muS)*distance);

betatotal=betarays*exp((-muH-muO-muN-muC-muS)*distance);

matrix(c,3)=alphatotal; matrixbeta(c,3)=betatotal;
```

A.3   Hair Dimensions

```
% David Silvers   Started: 9 February 2007   Completed:

% Writing code to scan the hair and slice it into slices.

% Take 5: 7 March 2007 This also finds the distance the x-ray

% travels through the hair.

function [a,delta,b,squarearea,roundarea,error]=slices(diameter,N)

radius=diameter/2; delta=(diameter+2)/N;

area=delta.^2; % Cross sectional area of a slice

a=zeros(N,N); x=a; y=a; for n=1:N

    for m=1:N

        x(n,m)=(n-ceil(N/2))*delta;

        y(n,m)=(m-ceil(N/2))*delta;

    end

end a=zeros(N,N); for n=1:N

    for m=1:N

        if x(n,m)^2 + y(n,m)^2 >= (radius-4)^2 && x(n,m)^2 + y(n,m)^2 <= (radius)^

          j=0;

          for i=1

              x1=x(n,m) + (x(n+1,m+1) - x(n,m))*rand;

              y1=y(n,m) + (y(n+1,m+1) - y(n,m))*rand;

                  if x1^2 + y1^2 <= radius^2

                      j=j+1;

                  end

          end

          if j>=1
```

```
                finder=1;
            else
                finder=0;
            end
            a(n,m)=finder;
        end
    end
end for n=1:N
    for m=1:N
        if x(n,m)^2 + y(n,m)^2 <= (radius-3)^2
            a(n,m)=5;
        end
    end
end k=1; for n=1:N
    for m=1:N
        if a(n,m) == k && a(n,m+1) ~= 0
            a(n,m+1) = k+1;
            k=k+1;
        end
        if m==N
            k=1;
        end
    end
end p=0; for n=1:N
    for m=1:N
        if a(n,m)~= 0
```

```
            p=p+1;
        end
    end
end squarearea=p*area; roundarea=pi*radius^2;
error=(1-squarearea/roundarea)*100; xtravel=0; b=zeros(N,N); for
n=1:N
    for m=1:N
        if a(n,m)~=0
            k=1;
            xtravel=0;
            for i=n:N
                if a(i,m)~=0
                    k=k+1;
                    xtravel=xtravel+1;
                    b(n,m)=xtravel;
                end
            end
        end
    end
end
```

A.4 Stop Power

```
% David Silvers  14 March 2007
% This calculates the stopping power. Refer to Table A8
function E=stoppower(E,delta) global powers
```

```
rhoHair=1.370; % units of g/cm^3

rhoH=.075*rhoHair; rhoO=.282*rhoHair; rhoN=.136*rhoHair;

rhoC=.46*rhoHair;

rhoS=.047*rhoHair; %.038-.082

Zn=1; %This is the atomic number for the element in question.

%Hydrogen

Sl=powers(Zn,2)*E^powers(Zn,3) + powers(Zn,4)*E^powers(Zn,5);

Sh=powers(Zn,6)/(E^powers(Zn,7))*log(powers(Zn,8)/E +

powers(Zn,9)*E); SEH=Sl*Sh/(Sl + Sh)*602.22/powers(Zn,10);

%Carbon

Zn=2; Sl=powers(Zn,2)*E^powers(Zn,3) + powers(Zn,4)*E^powers(Zn,5);

Sh=powers(Zn,6)/(E^powers(Zn,7))*log(powers(Zn,8)/E +

powers(Zn,9)*E); SEC=Sl*Sh/(Sl + Sh)*602.22/powers(Zn,10);

%Nitrogen

Zn=3; Sl=powers(Zn,2)*E^powers(Zn,3) + powers(Zn,4)*E^powers(Zn,5);

Sh=powers(Zn,6)/(E^powers(Zn,7))*log(powers(Zn,8)/E +

powers(Zn,9)*E); SEN=Sl*Sh/(Sl + Sh)*602.22/powers(Zn,10);

%Oxygen

Zn=4; Sl=powers(Zn,2)*E^powers(Zn,3) + powers(Zn,4)*E^powers(Zn,5);

Sh=powers(Zn,6)/(E^powers(Zn,7))*log(powers(Zn,8)/E +

powers(Zn,9)*E); SEO=Sl*Sh/(Sl + Sh)*602.22/powers(Zn,10);

%Sulfur

Zn=5; Sl=powers(Zn,2)*E^powers(Zn,3) + powers(Zn,4)*E^powers(Zn,5);

Sh=powers(Zn,6)/(E^powers(Zn,7))*log(powers(Zn,8)/E +

powers(Zn,9)*E); SES=Sl*Sh/(Sl + Sh)*602.22/powers(Zn,10);

% Since I input my hair in terms of microns, I need to divide by 10.
```

```
dEH=SEH*rhoH*delta/10; dEO=SEO*rhoO*delta/10; dEN=SEN*rhoN*delta/10;

dEC=SEC*rhoC*delta/10; dES=SES*rhoS*delta/10;

E=E-dEH-dEO-dEN-dEC-dES;
```

A.5   Attenuated x rays

```
% 16 March 2007    David Silvers

% Finding the numer of x-rays produced inside a cell of hair

% First, find the number of ionizations for this nonzero square

function [numbers,c,numbersbeta]=xrays(delta,distance,E,protons)

global numbers1 global numbersbeta1 global dense global practice2

global moles global flour1 rhoHair=1.370;

lengthx=length(practice2(:,1));          %Finds the number of rows

lengthy=length(practice2(1,:));          %Finds the number of columns

practice3=zeros(lengthx,lengthy+1);      %Puts in a column of zeros

practice3(:,1)=practice2(:,1);

practice3(:,3:lengthy+1)=practice2(:,2:lengthy); for Z=11:60

    Z1=Z - 9;                            %This matches the atomic number with t

    Z2=Z-10;

    vector=practice3(Z1,2:lengthy+1);      % Interpolates for different energies

    xdata=practice3(1,2:lengthy+1);

    ydata=vector;

    xinterp=0:1:practice3(1,lengthy+1);

    yinterp=interp1(xdata,ydata,xinterp,'cubic');  %These are the areas.

if E>0

    sigma=yinterp(floor(E)+1)*10^(-24);    % Cross-section found for element Z
```

```
else

    sigma=0;

end

    rho=dense(Z2,2)*rhoHair*10^(-6); % g/cm^3

    mole=moles(Z2,2); % This is the molar mass (g/mol) for element Z

    NA=6.023e23;        % Avogadro's Number (#/mol)

    ions=protons*rho*delta*10^(-4)/mole*NA*sigma;

    c=Z2;

    Kalpha=flour1(c,3);    %I'm just going to take the first energy, since the weig

                             % I can put in an average later if I so desire.

                             % Just get it running for now.

    Kbeta=flour1(c,5);     % Same thing with Kbetas. Worry about averages later. Ge

    omegaK=flour1(c,8);

    ratio=flour1(c,9);

    rays=ions*omegaK; % This is the number of ionizations that produce an x-ray.

    % Find out how many of those x-rays are Kalpha rays. Use 1/(1+ratio);

    alpharays=rays/(1+ratio);

    betarays=ratio/(1+ratio)*rays;

    %Find out how many of those rays get attenuated.

    numbers1(c,1)=Z;

    numbers1(c,2)=Kalpha;

    numbersbeta1(c,1)=Z;

    numbersbeta1(c,2)=Kbeta;

    [matrix, matrixbeta]=attenuation(distance,alpharays,betarays,Kalpha,Kbeta,c);

    numbers=numbers1+matrix;

    numbersbeta=numbersbeta1 + matrixbeta;
```

```
end
```

A.6   Thin Target x rays

```
% 16 March 2007    David Silvers

% Finding the numer of x-rays produced inside a cell of hair

% First, find the number of ionizations for this nonzero square

function [numbers1na,c,numbersbeta1na]=xraysthin(delta,E,protons)

global numbers1na global numbersbeta1na global dense global

practice2 global moles global flour1 rhoHair=1.370;

lengthx=length(practice2(:,1));          %Finds the number of rows

lengthy=length(practice2(1,:));          %Finds the number of columns

practice3=zeros(lengthx,lengthy+1);      %Puts in a column of zeros

practice3(:,1)=practice2(:,1);

practice3(:,3:lengthy+1)=practice2(:,2:lengthy); for Z=11:60

    Z1=Z - 9;                            %This matches the atomic number with t

    Z2=Z-10;

    vector=practice3(Z1,2:lengthy+1);       % Interpolates for different energies

    xdata=practice3(1,2:lengthy+1);

    ydata=vector;

    xinterp=0:1:practice3(1,lengthy+1);

    yinterp=interp1(xdata,ydata,xinterp,'cubic');  %These are the areas.

    sigma=yinterp(floor(E)+1)*10^(-24);    % Cross-section found for element Z

    rho=dense(Z2,2)*rhoHair*10^(-6); % g/cm^3

    mole=moles(Z2,2); % This is the molar mass (g/mol) for element Z

    NA=6.023e23;       % Avogadro's Number (#/mol)
```

```
ions=protons*rho*delta*10^(-4)/mole*NA*sigma;

c=Z2;

Kalpha=flour1(c,3);

Kbeta=flour1(c,5);

omegaK=flour1(c,8);

ratio=flour1(c,9);

rays=ions*omegaK; % This is the number of ionizations that produce an x-ray.

% Find out how many of those x-rays are Kalpha rays. Use 1/(1+ratio);

alpharays=rays/(1+ratio);

betarays=ratio/(1+ratio)*rays;

%Find out how many of those rays get attenuated.

numbers1na(c,1)=Z;              %na is not attenuated

numbers1na(c,2)=Kalpha;        %Before publishing, redo some of these variable n

numbersbeta1na(c,1)=Z;

numbersbeta1na(c,2)=Kbeta;

numbers1na(c,3)=alpharays;

numbersbeta1na(c,3)=betarays;

end
```