Summer Student
Programme 2008

July 23rd till
September 16th

Layout of materials and dimensions for the attenuator at petra III beamline BL8

Christian Geisler[γ] and Stanislav Gurskiy[μ]

supervised by

Dr. H. Oliver Seeck

[γ] Georg-August-Universität Göttingen
[μ] Lomonosov Moscow State University

The work presented in this document is the combined work of Stanislav Gurskiy and Christian Geisler during the course of the Desy Summer Programme 2008. Anyhow this document is split into three parts. The first part containing the choice of materials and thicknesses based on the most simple model of attenuation and was created in collaboration. The parts two and three deal with higher order corrections and represent the line of thought of the individual author. Due to limited time it was unfortunately impossible to thoughtfully compare the two approaches in this document.

Contents

1 Introduction

In this paper we will peresent the work we have done during the Desy Summer Student Programme 2008 in the team of Oliver Seeck who is the beamline scientist for the high resolution beamline at the PETRA III source.

The high brilliance synchrotron radiation source PETRA III will go in operation in 2009 with 14 beamlines each of them specialized to an x–ray method. Beamline 8 (BL 8, HighRes) is designed for high resolution diffraction and scattering experiments. It will deliver x-ray beams of a selected photon energy between 5KeV and 30KeV and a flux of up to 10^{15}cts/sec in the final stage.

2 The attenuator

The beam will have an intensity up to $I_{max} = 10^{15}$ photons per second whereas the utilized scintillator detector can only withstand up to $I = 10^5$ photons per second. This leads to the need of an attenuator which can reduce the photon flux. The attenuator device that will be used in the hires beamline is a device that slides 12 foils of different materials and thicknesses into the beam. In contrast to an attenuator wheel it will therefore be possible to combine the foils in $2^{12} = 4096$ ways which leads to a precise tuning of the attenuation factor.

3 Attenuation factor

The attenuation factor is defined as the quotient of the intensity of the incident beam and the transmitted beam:

$$\gamma = I/I_0 \tag{1}$$

The optimal attenuator would be in a binary setup, meaning that each foil absorbs twice as much intensity as the one before. If the foil i has an attenuation factor of γ_i then the binary setup corresponds to the recursive form:

$$\gamma_{i+1} = {\gamma_i}^2 \tag{2}$$

The attenuation will be highest when all 12 foils are pushed into the beam:

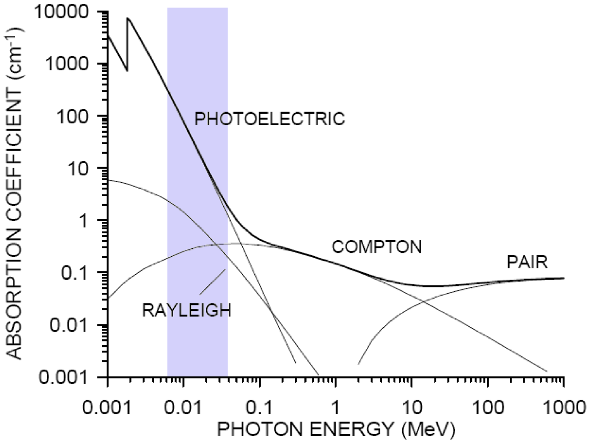
$$\gamma_{max} = \prod_{i=1}^{12} \gamma_i = {\gamma_1}^{\sum_{n=0}^{11} 2^n} = {\gamma_1}^{(2^{12}-1)}$$

With the highest absorption being equal to $I/I_{max} = 10^{-10}$ equation (3) can be solved for γ_1 and with relation (2) every γ_i can be derived recursively.

$$\begin{aligned} \gamma_1 &= \sqrt[4095]{10^{-10}} \approx 0.9944 & (3) \\ \gamma_i &= {\gamma_1}^{\sum_{n=0}^{i-1} 2^n} & (4) \end{aligned}$$

Beer-Lambert law – The Transmittance of radiation through a material can be approximated through the law of Lambert. This model considers the material as fully

Figure 1: Interaction of photons with Si



homogeneous. The particles in the material have the cross section σ and the number density ρ.

The operational cross-section σ is defined as:

$$\sigma(h\nu) = P(h\nu)/I(h\nu)$$

where P is the number of photons with the energy $h\nu$ absorbed per atom per unit time and I is the incident photon flux.

The fraction of photons absorbed per area by a slice of the material with thickness dz will therefor be $\sigma\rho dz$. That leads to the differential equation:

$$\frac{dI_z}{I_z} = -\sigma\rho dz$$

Integration via the length of the path leads to Lambert's law:

$$\begin{aligned} \ln(I_z) &= -\sigma\rho z + c \\ \ln(I_0) - \ln(I) &= -\sigma\rho l \\ \Rightarrow \qquad I/I_0 &= \exp(-\sigma\rho l) \qquad (5) \end{aligned}$$

In this context it is useful to introduce the absorption length $\lambda = 1/\sigma\rho$ and the absorption coefficient $\mu = \sigma\rho$ of a material. The absorption length is also the length after which the intensity of the radiation has decreased like $1/e$.

Photo ionization – In the energy range of 5.4KeV to 30KeV the photo ionization is the dominant interaction of photons with matter (cf. Figure 1) and will therefore determine the attenuation γ_i of the foils in the attenuator of the hires beamline at Petra III. In the process of photo ionization the total energy of a photon is absorbed by the electron shell of the atom. This effect occurs if the energy of the photon $h\nu$ is higher than the binding energy E_B of an electron in the shell. The photon then may excite an electron into the continuum and the excess energy $E_{kin} = h\nu - E_B$ will be transmitted as kinetic energy of the electron. If the frequency ν is high enough, the energy of the photon is sufficient not only to ionize the valence electrons but also the inner core electrons. With increasing energy more shells are effected by the photo ionization. This results in a characteristic absorption edges as soon new shells are attacked.

This phenomenon is similar to the photoelectric effect that occurs on the surface of solids.

(chart with absorption edges, figure with lambda, mass absorption coefficient, change due to impurity)

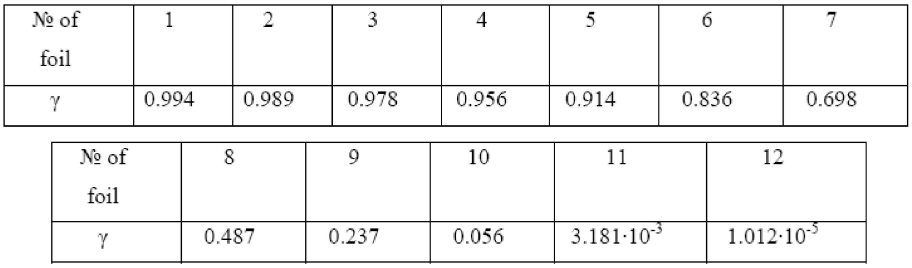
4 Choosing of materials for the attenuator

When choosing materials for the attenuator foils one should escape fluorescence from these materials when the attenuator foils are under the x-ray beam. In our case the attenuator should work in energy range from $5.4KeV - 30KeV$. The main problem is that absorption edge energy of chosen material should be bigger than energy of falling x-rays or at least should be less than 50% of falling x-rays to get rid of material fluorescence. Also due to the ability of x-ray beam to disperse while coming threw material maximal width of one foil should not be more than $1mm$. These two conditions restricted us in our choice of materials for the attenuator foils and their thicknesses.

We decided to choose aluminum first. Aluminum has absorption edge at $1.559KeV$, so there will be practically no fluorescence coming form foils made from aluminum.

To calculate thicknesses of aluminum foils we considered first all impurities in real aluminum foils and how they influence absorption length. According to Goodfellow company products we took aluminum with 99.0% purity (by mass weight). It contains 1000 Cu ppm, 7000 Fe ppm, 1000 Mn ppm, 5000 Si ppm and 1000 Zn ppm (ppm is given in weight ppm). This corresponds to co compound formula Al0.99057Cu0.042Fe0.335Mn0.049Si0.476Zn0.041. So having special program software we calculated absorption length for this composition depending on energy (cf. figure 2). As far as we calculated gammas γ_i for each foil for the highest possible energy of x-ray beam ($30KeV$) (cf. figure 3), we obtained that thicknesses of foils (cf. figure 4) should be as follows:

Figure 3: Calculated gammas for foils (30KeV).



№ of foil	1	2	3	4	5	6	7
γ	0.994	0.989	0.978	0.956	0.914	0.836	0.698

№ of foil	8	9	10	11	12
γ	0.487	0.237	0.056	$3.181\cdot10^{-3}$	$1.012\cdot10^{-5}$

Figure 2: Absorption length of aluminum as a function of photon energy.

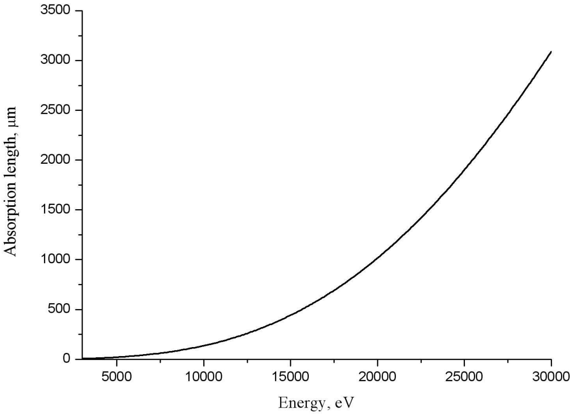
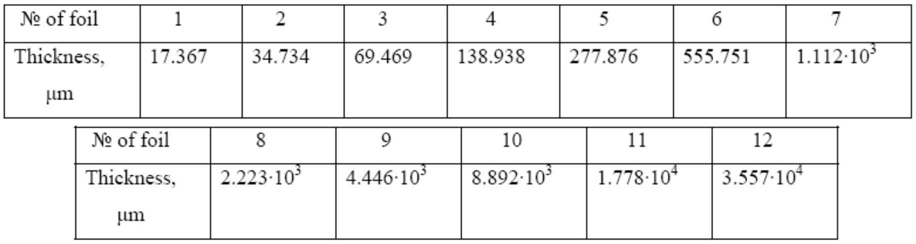


Figure 4: Calculated thicknesses of aluminum foils.

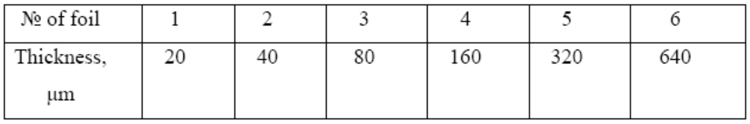


№ of foil	1	2	3	4	5	6	7
Thickness, µm	17.367	34.734	69.469	138.938	277.876	555.751	$1.112\cdot10^3$

№ of foil	8	9	10	11	12
Thickness, µm	$2.223\cdot10^3$	$4.446\cdot10^3$	$8.892\cdot10^3$	$1.778\cdot10^4$	$3.557\cdot10^4$

As we cannot use foils with thickness more than $1mm$, for 7th – 12th foils we had to use other materials to gain the same values of γ_i but thicknesses less than $1mm$. For first seven foils we chose thicknesses of foils according to Goodfellow company products (cf. figure 5):

Figure 5: Thicknesses of aluminum foils.



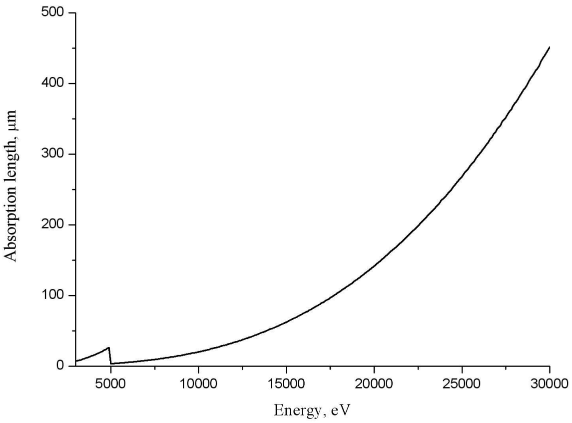
№ of foil	1	2	3	4	5	6
Thickness, µm	20	40	80	160	320	640

Maximal x-ray energy at which we are able to attenuate 10^{-10} of incoming intensity with the help of only first seven aluminum foils is $7.273KeV$. So in energy range $5.4KeV - 7.273KeV$ we will use only first seven foils made of aluminum.

As absorption edge of titanium is $4.966KeV$, it is convenient to use this metal as a material for next few foils because when using it for energies more than $7.273 KeV$ one cannot be afraid to obtain strong fluorescence from titanium foils.

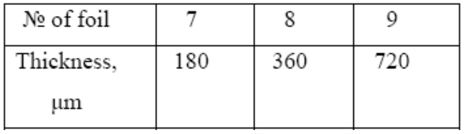
According to Goodfellow company products we took titanium with 99.6% purity (by mass weight). It contains 300 Al *ppm*, 20 Ca *ppm*, 50 Cr *ppm*, 5 Cu *ppm* and 1500 Fe *ppm*, 100 Mn *ppm*, 50 Ni *ppm*, 300 Si *ppm*, 200 Sn *ppm*, 300 C *ppm*, 60 H *ppm*, 150 N *ppm* and 2000 O *ppm* (*ppm* is given in weight *ppm*). With the help of special program software we calculated absorption length for real (impure) titanium foil depending on energy (cf. figure 6).

Figure 6: Absorption length of titanium as a function of photon energy.



According to Goodfellow company products we chose thicknesses of 7th, 8th and 9th titanium foils (cf. figure 7) as follows:

Figure 7: Thicknesses of titanium foils.



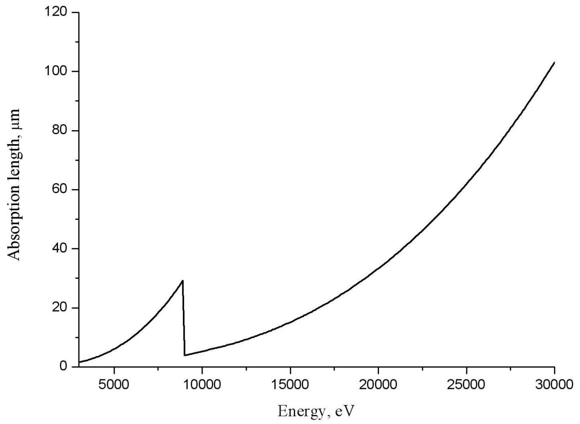
№ of foil	7	8	9
Thickness, µm	180	360	720

To gain value of attenuation 10^{-10} we can use our 9 foils for energy less or equal to $15.000 KeV$.

At last we should choose materials for 11th and 12th foils. It seemed for us that it will be reasonable to use copper for these foils because it has absorption edge at $8.979 KeV$ which is far away from $15.000 KeV$, copper is strong to corrosion (for example iron has absorption edge $7.112 KeV$, which is even more desirable than copper, but iron is well oxidized in oxygen atmosphere), also copper is ecologically safe (for example in comparison with cobalt) and rather cheap.

To calculate thicknesses of copper foils we considered first all impurities in real copper foils and how they influence absorption length. According to Goodfellow company products we took copper with 99.9% purity (by mass weight). It contains 500 Ag *ppm*, less than 10 Bi *ppm*, less than 50 Pb *ppm*, 400 O *ppm* (*ppm* is given in weight *ppm*). So having special program software we calculated absorption length for this composition depending on energy (cf. figure 8).

Figure 8: Absorption length of copper as a function of photon energy.



According to Goodfellow company products we chose thicknesses of 10th, 11th and 12th copper foils (cf. figure 9) as follows:

Figure 9: Thicknesses of copper foils.

№ of foil	10	11	12
Thickness, μm	320	640	1280

Now when using all chosen foils for energy of incoming x-ray beam $30 KeV$ we can gain maximal value of $\gamma = 1.510^{-11}$, which is even more than we have planned.

5 Computing the combination

To obtain the appropriate combination of foils for a desired attenuation a Java program has been developed. The major steps in the process are the listed:

1. The program reads the materials, thicknesses and positions of the foils utilized in the attenuator from a file ("setup.txt").

2. For a given photon energy it interpolates from tabulated values the absorption length for each material and calculates the absorption factor γ_i for each foil i.

3. Via comparing the absorption using a different foil combination the combination and the corresponding absorption which is the closest to the desired attenuation is the output.

In following the different methods utilized in the program ”absorption.java” are briefly explained. The full code can be found in the appendix.

– *readIn()* reads in the first 9 characters of the *i*th line of the ASCII file ”setup.txt” as thickness of foil i made out of the material with characters 10 and 11 (e.g. ”1280e-6 Cu”). The setup is stored in a string-array holding the materials and a double array holding the thickness.

– *getLambda(energy,material)* returns the interpolated values for the absorption length in microns for a given energy and material. The tabulated values have to be in a file named ”material”.

– *makeLambdaArray(energy)* creates a double a double array holding the absorption length λ_i of each foil. It uses the arrays previously created by readIn().

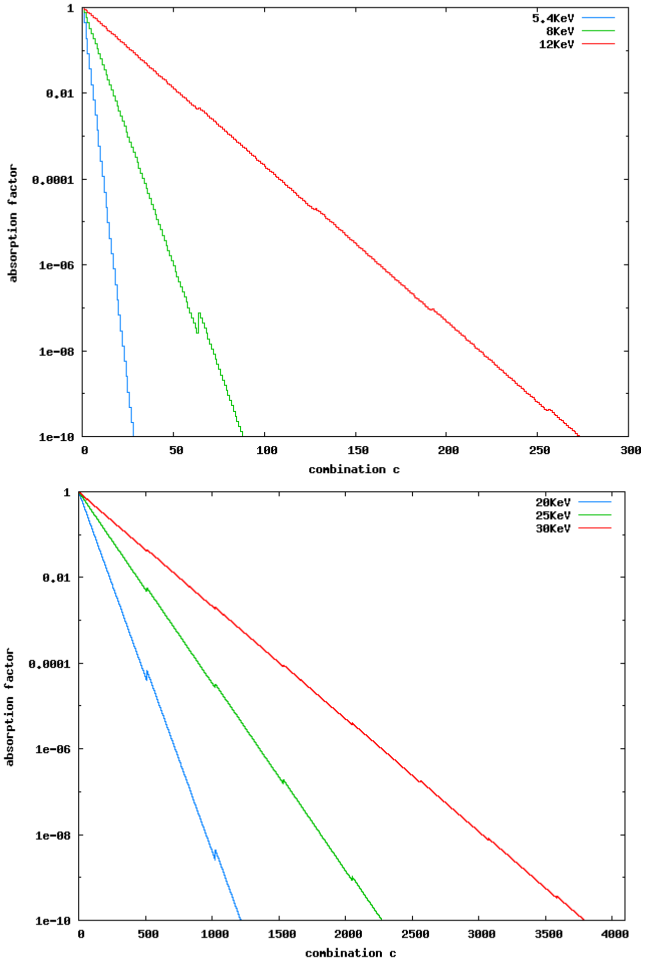
– *toBinary()* converts an decimal integer $0 \leq c \leq 4095$ to a binary array. This makes it possible to convert a number to a combination of inserted and withdrawn foils. This is done so that c increases with the attenuation of the combo.

– *calculateGamma(c)* calculates the absorption γ_c of the combination c.

– *getCombo(γ,energy)* compares the gamma for combination $c = 0$ with the desired combination. If γ_c of the combo c is larger than γ then c and γ_c are returned in a string array. Else the procedure is repeated with $c = c + 1$.

With the use of the Java code the attenuation γ can be calculated for a given photon energy as a function of the combination c. These calculations are illustrated in figure 10. The deviations from the linear behavior are due to the change in material used to absorb photons.

Figure 10: The absorption factor I/I_0 depends on the combination of foils slid into the beam. Displayed here is the course of γ in the low and high energy range.



References

[YEH] J.-J. Yeh, Atomic Calculation of Photoionization Cross-Sections and Asymmetry Parameters, Gordon and Breach

[LeRa] Claude Leroy and Pier-Giorgio Rancoita, Principles of Radiation Interaction in Matter Detection

[Ash] Ashcroft and Marmin, Solid State Physics

A Code ”absorption.java”

```
import java.util.*;
import java.math.*;
import java.io.*;

public class absorption{
    static String OutputFile;
    static double[] Thickness = new double[12];
    static String[] Material = new String[12];
    static double[] Lambda = new double[12];
    static String setup = "setup.txt";

    static void readIn() throws Exception{
        FileReader fr = new FileReader(setup);
        BufferedReader br = new BufferedReader(fr);
        String line = null;
        for(int i = 0 ; i<=11 ; i++) {
            line = br.readLine();
            Thickness[i] = Double.parseDouble(line.substring(0,8));
            Material[i] = line.substring(9,11);
        }
        fr.close();
        br.close();
    }

    static double getLambda(double Energy, String material) throws Exception{
        FileReader fr = new FileReader(material);
        BufferedReader br = new BufferedReader(fr);
        for(int i=0 ; i<5 ; i++) br.readLine();
        String line2;
        String line1 = "null";
        Double E1, E2, L1, L2;
        while((line2=br.readLine())!="null"){
            try{
                if((E2=Double.parseDouble(line2.substring(0,10))) <= Energy){
                    line1=line2;}
                else{
                    E1=Double.parseDouble(line1.substring(0,10));
                    L1=Double.parseDouble(line1.substring(54,line1.length()));
                    L2=Double.parseDouble(line2.substring(54,line2.length()));
                    return( L1+((L1-L2)/(E1-E2))*(E1-Energy) );}
            }
            catch(NumberFormatException e){;}
        }
```

```
        return(0.0);
    }

    static void makeLambdaArray(Double Energy) throws Exception{
        double l = 0;
        String m = "";
        for(int i=11 ; i>=0 ; i--){
            if (Material[i].compareTo(m)==0) Lambda[i]=l;
            else{
                Lambda[i]=getLambda(Energy, Material[i]);
                l = Lambda[i];
                m = Material[i];
            }
        }
    }

    public static int[] toBinary(int C){
        int[] BC = new int[12];
        int d = 2048;
        for(int i=11; i>=0 ; i--){
            if (C >= d) BC[i] = 1;
            else BC[i] = 0;
            C=C%d;
            d=d/2;}
        return(BC);
    }

    public static double calculateGamma(int C) throws Exception{
        int[] BC = toBinary(C);
        double e = 0;
        for(int i = 11 ; i>=0 ; i--){
            e = e+((BC[i]*Thickness[i])/(Lambda[i]*1e-6));
        }
        return(Math.exp(-e));
    }

    public static String[] getCombo(double gamma, double Energy) throws Exception{
        readIn();
        makeLambdaArray(Energy);
        String[] a = new String[2];
        for(int c=0 ; c<4096 ; c++){
            if(gamma > calculateGamma(c)){
                a[0]=Double.toString(calculateGamma(c));
                a[1]=Integer.toString(c);
                return(a);
            }
        }
        return(a);
    }

    public static void main(String[] A) throws Exception{
        BufferedReader br = new BufferedReader( new InputStreamReader(System.in));
        System.out.print("Desired absorption: ");
        double gamma = Double.parseDouble(br.readLine());
        System.out.print("What is the energy of the beam [eV]: ");
        Double Energy = Double.parseDouble(br.readLine());
        String[] a = getCombo(gamma,Energy);
```

```java
        int[] b = toBinary(Integer.valueOf(a[1]));
        System.out.print(a[0]+"\t");
        for(int i=0; i<b.length; i++)    System.out.print(b[i]);
        System.out.println();
    }
}
```

6. Higher order corrections (made by Stanislav Gurskiy)

When calculating attenuation coefficients (gammas) and consequently thicknesses for attenuator foils one should always take in to consideration two factors: x-ray bragg scattering from foils due to its grain nature and fluorescence coming from foils.

In this section we will pay all attention to scattering of intensity and will not consider fluorescence because we were short of time to cover both of these two problems.

So we will consider bragg scattering within foils to know how much intensity we will loose after x-ray beam will pass threw foils.

6.1. Bragg scattering

It is commonly known that usually foils of various materials consist of grains [1]. For commercial foils mean grain size is varied between 0.2 and 2.5 μm. Distribution of these grains in space of foil depends on way to obtain foil and on its thickness but still remains practically equiaxed (i.e. random). These grains are small crystals so the whole volume of foil is actually a powder which consists of very large number of small crystallites. Consequently there will be bragg scattering of incoming x-ray beam on these crystallites. To characterize this phenomenon quantitatively we applied x-ray powder diffraction theory. If we are dealing with imperfect crystallites (as in our case) than diffraction from these crystallites is well described with kinematic theory of diffraction. This is due to real structure of crystallites. Such a crystallite represents a mosaic of crystal blocks about 10^{-7} m in size [2], which are more or less misoriented with respect to each other by angles of the order of fraction of minute [2]. Such a crystallite is called ideally mosaic. The coherent interactions of scattered waves in such a crystallite occurs within a single block. As for scattering by a mosaic crystallite as a whole, it is defined by the sum of intensities of scattering by each block.

To calculate intensity scattered by a foil we should use following approximations.

Integrated intensity of reflection hkl (I_{hkl}), scattered from one block is given by equation (1) [3]:

$$I_{hkl} := I_0 \cdot k_1 \cdot k_2 \cdot p_{hkl} \cdot L_\theta \cdot P_\theta \cdot A_\theta \cdot T_{hkl} \cdot E_{hkl} \cdot \left(\left|F_{hkl}\right|\right)^2 \cdot N^2 \qquad (1)$$

where I_0 is incoming intensity; $k_1 = (r_e)^2$, r_e is classical electron radius ($r_e = 0.28178 \cdot 10^{-12}$ m); $k_2 = (\lambda^3/V_{cell})$, V_{cell} is volume of elementary cell; p_{hkl} is multiplicity factor which equals to number of symmetrically equivalent (hkl) planes; $L_\theta P_\theta$ is Lorentz-polarization factor which accounts for polarization of incoming beam and geometry of experiment; A_θ is absorption of intensity inside block; T_{hkl} is factor of preferred orientation of blocks in illuminated volume concerning (hkl) planes; E_{hkl} is extinction factor; $N = V_{block}/V_{cell}$ is number of elementary cells in one block; F_{hkl} is structure factor:

$$F_{hkl} := \sum_j \left[t_j \cdot f_j \cdot \exp\left[2\pi i \cdot \left(h \cdot x_j + k \cdot y_j + l \cdot z_j\right)\right]\right] \qquad (2)$$

where sum is taken over all atoms in elementary cell. In formula (2) t_j is Debye-Waller temperature factor, f_j is atomic scattering factor (in electrons per atom). Debye-Waller temperature factor in case of isotropic atomic movements is given by the formula 3:

$$t_j := \exp\left[-B_j \cdot \left(\frac{\sin(\theta)}{\lambda}\right)^2\right] \qquad (3)$$

where $B_j = 8\pi^2 \cdot (U_{x\,j})^2$ and $U_{x\,j}$ is root mean square deviation of j^th^ atom from its equilibrium position (x,y,z) in x-direction (in Å).

When (hkl) planes within blocks from different crystallites diffract, they produce diffraction circle appropriate to (hkl) series of planes. So we will have whole number of allowed (hkl) diffraction circles with certain width. Let's assume that each of these circles has the same width Δ. The variety (w) that a certain grain will hit infinitively thin circle, which has opening angle 2θ is given by equation (4):

$$dw(\theta) = 0.5 \cdot \cos(\theta) d\theta \quad (4).$$

Number of grains (N_{grains}) which will hit the whole diffraction circle with width Δ will be:

$$N_{grains} := \frac{V}{V_{grain}} \cdot \int_{\theta_{bragg} - 0.5\Delta}^{\theta_{bragg} + 0.5\Delta} 0.5 \cdot \cos(\theta)\, d\theta \qquad (5a)$$

which equals to

$$N_{grains} := \frac{V}{V_{grain}} \cdot 0.5 \cdot \cos\left(\theta_{bragg}\right) \cdot \sin(\Delta) \qquad (5b)$$

In equation (5)(a,b) V is illuminated area and V_{grain} is volume of single grain. As each grain has a mosaic structure which is a normal sharp distribution over θ_{bragg}, in range ($\theta_{bragg} - 0.5 \cdot \Delta$; $\theta_{bragg} + 0.5 \cdot \Delta$) will be situated about 95 % of blocks in each grain. So number of blocks N_{blocks} which will diffract and produce diffraction circle is:

$$N_{blocks} := 0.95 \cdot \frac{V_{grain}}{V_{block}} \cdot \frac{V}{V_{grain}} \cdot 0.5 \cdot \cos\left(\theta_{bragg}\right) \cdot \sin(\Delta) \qquad (6).$$

where V_{block} is volume of single block. Neglecting preferred orientation and extinction factors integrated intensity of (hkl) reflection is given by equation (7):

$$I_{hkl} := I_0 \cdot k_1 \cdot k_2 \cdot p_{hkl} \cdot L_\theta \cdot P_\theta \cdot A_\theta \cdot T_{hkl} \cdot E_{hkl} \cdot \left(\left|F_{hkl}\right|\right)^2 \cdot \left(\frac{V_{blocks}}{V_{cell}}\right)^2 \cdot 0.95 \cdot \frac{V_{grain}}{V_{block}} \cdot \frac{V}{V_{grain}} \cdot 0.5 \cdot \cos\left(\theta_{bragg}\right) \cdot \sin(\Delta) \tag{7}$$

Total diffracted integrated intensity is sum over all possible I_{hkl}:

$$\frac{I}{I_0} := \sum_{hkl} \frac{I_{hkl}}{I_0} \tag{8}$$

In this approximation we calculated dependence of I/I_0 on incoming x-ray beam energy for aluminum and copper foils. Illuminated volume V for each material (Table 6) was taken as area of beam multiplied by thickness of all foils made of this material $V = S \cdot d$, where S is cross-sectional area of incoming beam (which was taken 16 mm^2) and d is thickness of all attenuator foils made of certain material:

Table 6. Illuminated volume

Material	Al	Cu
Volume, m^3	$2.016 \cdot 10^{-8}$	$3.584 \cdot 10^{-8}$

We took $V_{block} = 10^{-21}$ m^3, $V_{grain} = 10^{-18}$ m^3, $\Delta = 1.74533 \cdot 10^{-5}$ radian. Values for V_{cell} for aluminum and copper are given in Table 7:

Table 7. Elementary cell volume

Material	Al	Cu
Volume, m^3	$66.381 \cdot 10^{-30}$	$47.242 \cdot 10^{-30}$

Atomic scattering factor curves for Al and Cu were obtained after approximation of data [4] by polynomial of six power:

$$f(x)_{Al} := 13 + (-13.39127) \cdot x + (-91.5025) \cdot x^2 + (466.83034) \cdot x^3 + (-915.01777) \cdot x^4 + (807.68356) \cdot x^5 + (-265.39086) \cdot x^6$$

$$f(x)_{Cu} := 29 + (-2.04843) \cdot x + (-211.43178) \cdot x^2 + (561.13841) \cdot x^3 + (-702.67577) \cdot x^4 + (453.47658) \cdot x^5 + (-120.3481) \cdot x^6$$

where x is $\sin(\theta)/\lambda$.

Lambda value for different photon energies is given by equation lambda (m) = 12.398/Energy(KeV)·10^{-10}.

Considering Debye-Waller temperature factor we assumed all atoms in metal crystal deviated isotropically form their positions. Values of root mean square deviation U_x of Al and Cu atoms in metal were taken from [4] for 290 °K (Table 8):

Table 8. Root mean square deviation of atoms in metal (290 °K)

Atom	Al	Cu
U_x, Å	0.099	0.085

To calculate values of I/I_0 for energies in the range 5.4 – 30 KeV program code was created using Mathcad 13.1 software was used. Calculation results for aluminum and copper are presented on Figure 1 and 2 correspondingly:

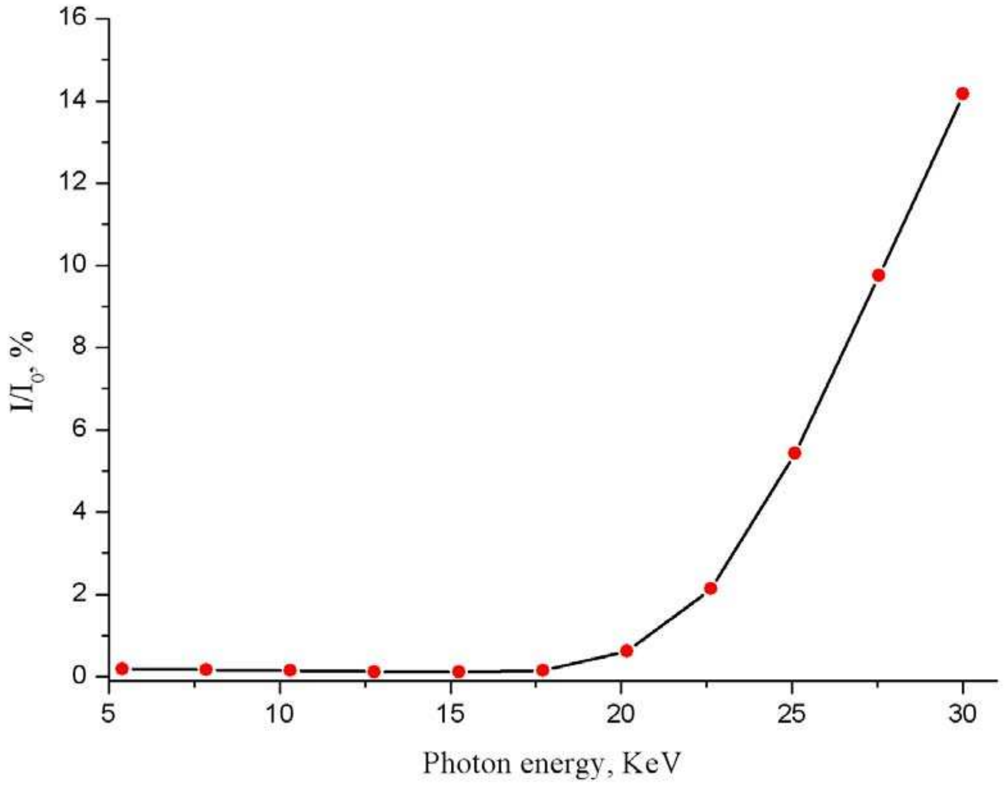


Figure 1. I/I_0 for all aluminum foils (thickness = 1.26 mm)

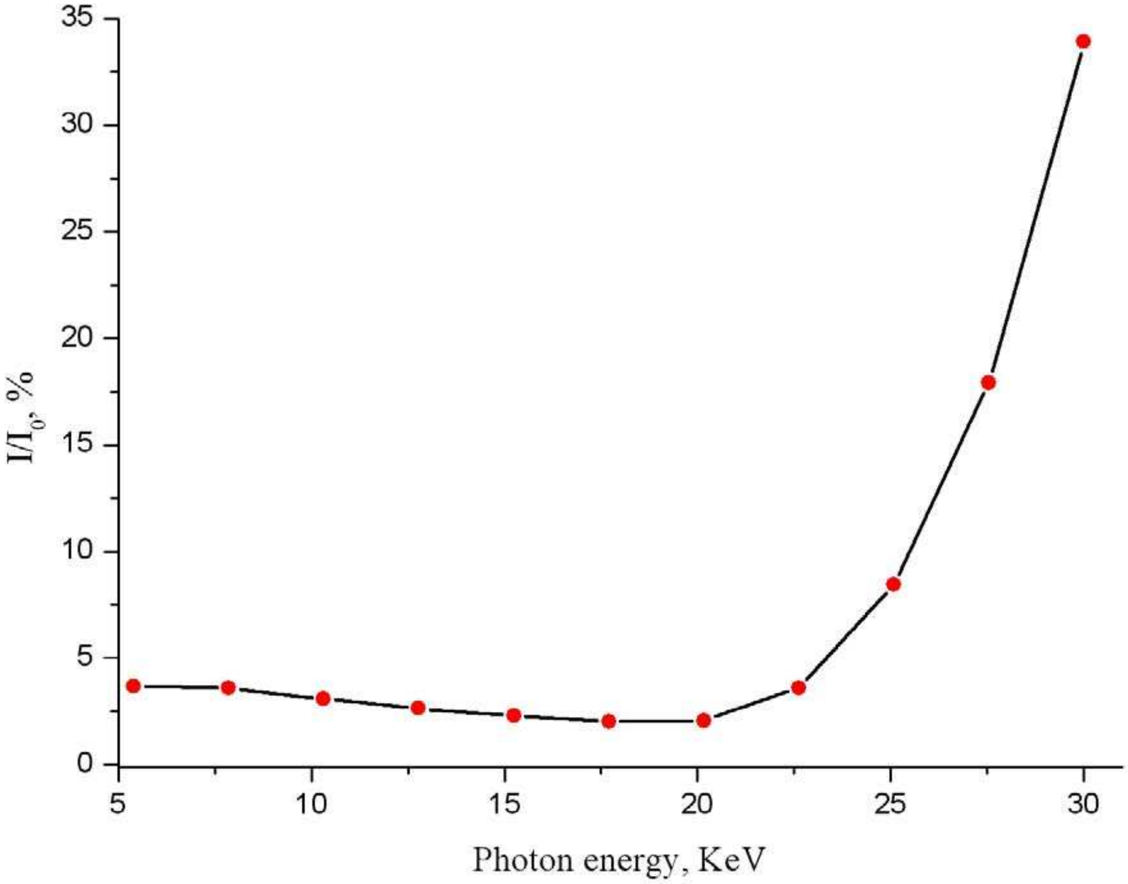


Figure 2. I/I$_0$ for all copper foils (thickness = 2.24 mm)

As shown on Figure 1 and Figure 2 I/I$_0$ has practically constant value in energy range between 5.4 KeV and 20 KeV and stars to increase rapidly with energies more than 20 KeV. One can explain such behavior because of influence of two factors on I/I$_0$. On the one hand with increase of energy number of possible reflections rapidly increases (proportional to $1/\lambda^3$) and on the other hand influence of this reflections on whole percentage of scattered intensity is rapidly decreasing due to scattering factor and Debye-Waller temperature factor. It can be so that if energy is lower than 20 KeV these three factors cancel each other and percentage of scattered intensity stays practically the same. But when energy is more than 20 KeV number of all possible reflections has more strong influence in comparison to scattering factor and Debye-Waller temperature factor.

6.2. Mathcad program code

In this section we will present code made in program package Mathcad 13.1 to calculate percentage of intensity, scattered from aluminum or copper foils. Presented code is written for aluminum which has cubic face centered elementary cell (space group Fm3m) with cell parameter 4.049 Å. For any other material with Fm3m symmetry (for example copper) the code is similar.

E

$$\lambda := \frac{12.398}{E} \cdot 10^{-10}$$

$$a := 4.049 \cdot 10^{-10}$$

$$Vcell := a^{3}$$

$$Vblock := 1 \cdot 10^{-21}$$

$$Vgrain := 10^{-18}$$

$$V := 2.01600 \cdot 10^{-8}$$

$$\Delta := 1.74533 \cdot 10^{-5}$$

$$u := 0.099$$

$$k1 := 7.94 \cdot 10^{-30}$$

$$k2 := \frac{\lambda^{3}}{Vcell}$$

$$f(x) := 13 + (-13.39127) \cdot x + (-91.50251) \cdot x^{2} + (466.83034) \cdot x^{3} + (-915.01777) \cdot x^{4} + (807.68356) \cdot x^{5} + (-265.39086) \cdot x^{6}$$

```
$HKL(E, n) :=$
    $j \leftarrow 0$
    $h \leftarrow 0$
    $k \leftarrow 0$
    $l \leftarrow 0$
    while $\frac{12.398}{2 \cdot E} \cdot \frac{\sqrt{h^2}}{4.049} \le 1$
        while $\frac{12.398}{2 \cdot E} \cdot \frac{\sqrt{h^2 + k^2}}{4.049} \le 1$
            while $\frac{12.398}{2 \cdot E} \cdot \frac{\sqrt{h^2 + k^2 + l^2}}{4.049} \le 1$
                while $\frac{12.398}{2 \cdot E} \cdot \frac{\sqrt{h^2 + k^2 + l^2}}{4.049} \le 1$
                    break if $\mathrm{mod}(h + k, 2) \ne 0$
                    break if $\mathrm{mod}(h + l, 2) \ne 0$
                    break if $\mathrm{mod}(l + k, 2) \ne 0$
                    $H_{j,0} \leftarrow h$
                    $H_{j,1} \leftarrow k$
                    $H_{j,2} \leftarrow l$
                    $j \leftarrow j + 1$
                    $l \leftarrow l + 1$
                $l \leftarrow l + 1$
            $k \leftarrow k + 1$
            $l \leftarrow 0$
        $h \leftarrow h + 1$
        $k \leftarrow 0$
    $H$ if $n = 0$
    $j - 1$ if $n = 1$
```

$A := \mathrm{HKL}(E,0)$

```
SIN(E) :=
    for  i ∈ 0..HKL(E,1)
        $B_i \leftarrow \frac{\lambda}{2}\cdot\sqrt{\frac{\left(A_{i,0}\right)^2+\left(A_{i,1}\right)^2+\left(A_{i,2}\right)^2}{a^2}}$
    B
```

$C := \mathrm{SIN}(E)$

```
formfactor(E) :=
    for  i ∈ 0..HKL(E,1)
        $y \leftarrow C_i$
        $D_i \leftarrow f\left(\frac{y}{\lambda\cdot 10^{10}}\right)\cdot\exp\left[-8\pi^2\cdot u^2\cdot\left(\frac{y}{\lambda\cdot 10^{10}}\right)^2\right]$
    D
```

$F := \mathrm{formfactor}(E)$

```
Θ(E) :=
    for  i ∈ 0..HKL(E,1)
        $G_i \leftarrow \mathrm{asin}\left(C_i\right)$
    G
```

$I := \Theta(E)$

```
Nproperblocks(E) :=
    for  i ∈ 0..HKL(E,1)
        $J_i \leftarrow \frac{V}{Vgrain}\cdot\frac{1}{2}\cdot\cos\left(I_i\right)\cdot\sin(\Delta)\cdot 0.95\cdot\frac{Vgrain}{Vcoherent}$
    J
```

$K := \mathrm{Nproperblocks}(E)$

```
Polarization(E) :=
    for i ∈ 1..HKL(E, 1)
        $L_i \leftarrow \frac{1 + \cos(I_i)^2}{4\cdot\cos(I_i)\cdot\sin(I_i)^2}$
    L
```

O := Polarization(E)

```
Strucfactor(E) :=
    for i ∈ 1..HKL(E, 1)
        $M_i \leftarrow 16\cdot\left(\frac{Vblock}{Vcell}\right)^2\cdot(F_i)^2$
    M
```

P := Strucfactor(E)

```
Multiplicity(E) :=
    for i ∈ 0..HKL(E, 1)
        $Q_i \leftarrow$
            8 if $A_{i,0} \neq A_{i,1} \neq A_{i,2} \neq A_{i,0}$
            8 if $A_{i,0} = A_{i,1} \neq A_{i,2}$
            8 if $A_{i,0} = A_{i,2} \neq A_{i,1}$
            8 if $A_{i,1} = A_{i,2} \neq A_{i,0}$
            4 if $A_{i,0} = A_{i,1} \neq A_{i,2} = 0$
            4 if $A_{i,1} = A_{i,2} \neq A_{i,0} = 0$
            4 if $A_{i,0} = A_{i,2} \neq A_{i,1} = 0$
            8 if $A_{i,0} = A_{i,1} = A_{i,2}$
            4 if $A_{i,2} = 0 \neq A_{i,0} \neq A_{i,1} \neq 0$
            4 if $A_{i,1} = 0 \neq A_{i,0} \neq A_{i,2} \neq 0$
            4 if $A_{i,0} = 0 \neq A_{i,1} \neq A_{i,2} \neq 0$
            2 if $A_{i,1} = A_{i,2} = 0 \neq A_{i,0}$
            2 if $A_{i,0} = A_{i,2} = 0 \neq A_{i,1}$
            2 if $A_{i,0} = A_{i,1} = 0 \neq A_{i,2}$
            4 if $A_{i,0} = 0 \neq A_{i,1} \neq A_{i,2} \neq A_{i,0}$
            0 if $A_{i,0} = A_{i,1} = A_{i,2} = 0$
    Q
```

R := Multiplicity(E)

```
$\mathrm{IoverIzerohkl}(E) :=$
    for $i \in 1 .. \mathrm{HKL}(E, 1)$
        $N_i \leftarrow k1 \cdot k2 \cdot R_i \cdot O_i \cdot P_i \cdot K_i$
    $N$
```

$$S := \mathrm{IoverIzerohkl}(E)$$

$$\mathrm{IoverIzeropercents} := 100 \cdot \sum_{k=0}^{\mathrm{HKL}(E,1)} S_k$$

6.3. Conclusion

Based on made calculations one can say that when using all aluminum and copper foils incident beam can loose maximum 40% (in case of energy of incident beam 30 KeV) of incoming intensity due to scattering on foil grains. However there still should be done experiments and qualitative measurements to prove or to dispruve these calculations.

6.4. Used literature

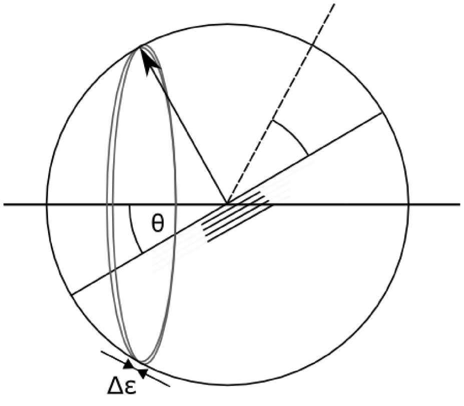
1) H. D. Merchant, W. C. Liu, L. A. Giannuzzi, J. G. Morris // *Materials Characterization*, 2004, 53, 335-360;

2) Boris K. Vainshtein // Fundamentals of crystals, New York, Springer, 1994, v. 1, P. 253;

3) V. K Pecharsky, P.Y. Zavalij // Fundamentals of powder diffraction and structural characterization of materials, New York, Springer, 2005, P. 187;

4) International Tables for Crystallography, 1985, V. 3, P. 233-239, P. 210-212.

Figure 1: The probability that a plane is in the right orientation depends on the acceptance angle $\Delta\varepsilon$ and the Bragg angle θ.



6 Higher order corrections (made by Christian Geisler)

The next order of correction to the attenuation of a metal foil comes from elastic coherent scattering of the photons on the crystallites in the foil.

6.1 Appreoach via "semi" dynamic theory

In this approach the Lambert-Beers law will be utilized in combination with published values for the extinctionlength for perfect crystalls in dynamic theory.

Bragg-condition – Bragg stated the condition for constructive interference from a set of planes in a crystal miller indexed with h,k and l which have an inter-planar distance d_{hkl} in dependence of the radiation wavelength λ and the scattering angle θ as:

$$2d_{hkl}\sin(\theta_{Bragg}) = \lambda. \tag{1}$$

Probability factor – A plane not illuminated under the acceptance of the Bragg angle $\theta_{Bragg} \pm \Delta\varepsilon$ it will not reflect photons. From figure 1 we see, that the probability p for a isotropically statistically oriented plane (hkl) to be in the right orientation for a reflection depends on the Bragg angle θ_{Bragg} of the plane and the acceptance width $\Delta\varepsilon$ like:

$$p = \frac{2\pi\cos(\theta_{Bragg})}{4\pi}\Delta\varepsilon \tag{2}$$

The probability factor therefore can be expressed as:

$$p = \frac{2\pi\cos(\arcsin(\lambda/2d_{hkl}))}{4\pi}\Delta\varepsilon \tag{3}$$

Geometrical structure factor – The amplitude of the scattered light is additionally altered by a geometrical structure factor S_K that accounts for the fixed positions of the atoms in the unit cell and the resulting constructive or destructive interference.

Let $\vec{K}$ be the difference between the wave vectors $\vec{k}'$ and $\vec{k}$. The difference in path for a wave scattered at $\vec{d_i}$ and $\vec{d_j}$ will then be $\vec{K}\cdot(\vec{d_i}-\vec{d_j})$ and the phase will differ by $\exp(i\vec{K}\cdot(\vec{d_i}-\vec{d_j}))$. The superposition of the individual rays from each center of scattering will give an amplitude containing the factor

$$S_{\vec{K}} = \sum_{j=1}^{n} \exp\left(i\vec{K}\cdot\vec{d_j}\right) \tag{4}$$

and the intensity will be proportional to $S_{\vec{K}}^2$ accordingly.

To calculate the geometrical structure factor of a fcc lattice be consider it a simple cubic lattice with a four-point-basis consisting of:

$$\vec{d}_1 = 0, \qquad \vec{d}_2 = \frac{a}{2}(\hat{e}_x+\hat{e}_y), \qquad \vec{d}_3 = \frac{a}{2}(\hat{e}_y+\hat{e}_z), \qquad \vec{d}_4 = \frac{a}{2}(\hat{e}_z+\hat{e}_x)$$

The vector of the cubic reciprocal lattice has the form

$$\vec{K} = \frac{2\pi}{a}(h\hat{e}_x + k\hat{e}_y + l\hat{e}_z).$$

Therefore the geometric structure factor becomes:

$$S_{\vec{K}} = \exp(i0) + \exp(i\pi(h+k)) + \exp(i\pi(k+l)) + \exp(i\pi(l+h)). \tag{5}$$

$S_{\vec{K}}$ will then will be 4 if h, k and l will all be either even or odd. In every other case it will equal 0.

Polarization factor – The probability to detect a scattered photon from the sample at a point on the unit sphere is proportional to the square of electric field amplitude E^2 in that point.

Lets consider a dipole in the position O and a Point on the unit sphere P. Let further be the incident beam identical to the z-axis fully polarized in the direction of the x-axis. Then the amplitude of the E-field depends only on the angle ϕ which is the angle between the zy-plane and the vector OS (cf. figure **??**). The apparent amplitude in any direction depending on ϕ is:

$$\hat{E} = \hat{E}_0 \cos\phi$$

In the following we use a Monte Carlo method to sum the amplitudes squared in all the points S that full fill the condition that the angle between OS and the z-axis is θ. This condition corresponds to all S on the unit sphere with:

$$S_z = \cos\theta$$

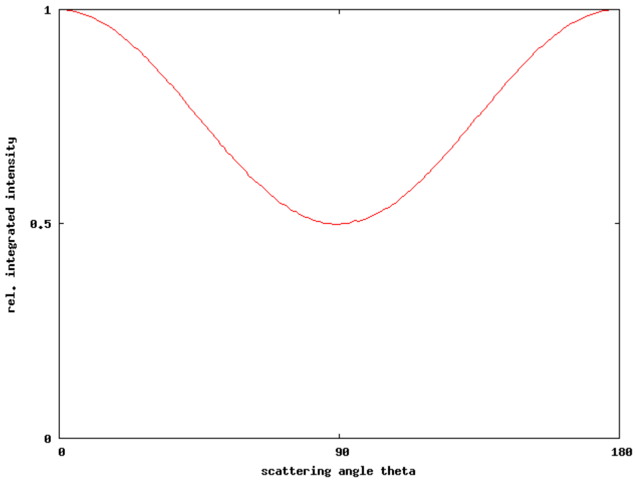
S is further linked to ϕ via:

$$S_x = \sin\phi$$

Using three random numbers (Ψ, Θ, Φ) a point S on the sphere is picked, its Cartesian coordinates are given through:

$$\begin{aligned}
S_x &= \cos(\Psi)\cos(\Phi) - \sin(\Psi)\cos(\Theta)\sin(\Phi)\\
S_y &= \sin(\Psi)\cos(\Phi) + \cos(\Psi)\cos(\Theta)\sin(\Phi)\\
S_z &= \sin(\Theta)\sin(\Phi)
\end{aligned}$$

Figure 2: Relative integrated intensity in dependence of the scattering angle obtained using 10^7 random points S and $n = 180$.



The range of θ is divided into n bins with width $\Delta = (\pi/n)$. Linked to each point S there is an angle θ which is assigned to bin i if θ is in $[(i-1)\Delta, i\Delta)$. After creating a large number of S the $\hat{E}^2$ for every S in the each bin is summed up and divided by the number of S in the bin. This value then represents the averaged integrated intensity for the averaged $\theta = (i-1/2)\Delta$ in bin i. The result obtained is plotted in figure 2 and corresponds to the analytical solution of [Warren]:

$$P = \frac{1+\cos^2\theta}{2} \tag{6}$$

Probability to scatter a photon – The probability W that a photon is scattered at a grain with a random and isotropic orientation the following formula is used:

$$W = \sum_h \sum_k \sum_l \qquad p(\theta(hkl)) \times S(hkl) \times P(\theta(hkl)) \times \exp(-\sigma_{photo} l) \times E(hkl) \tag{7}$$

The first three factors are explained in the corresponding sections above. $\exp(\sigma_{photo} l)$ is the factor that plugs the photo-ionic absorption into the balance. The factor E accounts for the fact that the cross-section of the symmetric Bragg-diffraction differs with inter planar distance of the deflecting planes.

Extinction – The extinction term holds the Bragg-cross-section in the form of:

$$E(hkl) = \exp(-l\ \sigma_{elastic}\rho) = \exp(-2l\ /\tau(hkl))$$

where τ is the extinction length of the plane hkl and l the length of the crystallites in $\hat{e}_z$.

The extinction length is the distance in a perfect crystal, after which the amplitude of the photon is reduced by $1/e$ and the intensity by $1/e^2$ accordingly. This value can be

Figure 3: Extinction length of Si (red points) from database and fit (green).

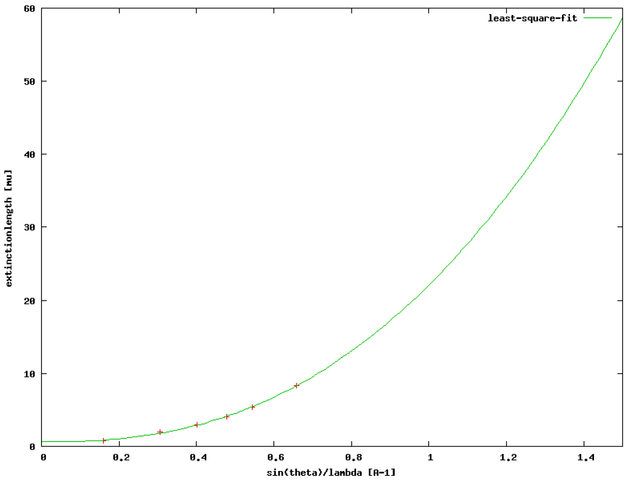
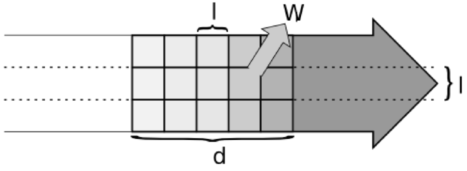


Figure 4: The probability to loose a photon on the path via the foil depends on the probability to scatter on one grain and on the number of grains in the path.



obtained for a perfect silicon Crystal from calculations with *X0h* a program accessible through the x-ray server at Argonne National Laboratory.

Since silicon has a similar qualities like aluminium it can be used to approximate the extinction lengths of the Al-foil.

The extinction length depends on the inter-planar distance d_{hkl} like (cf. figure 3):

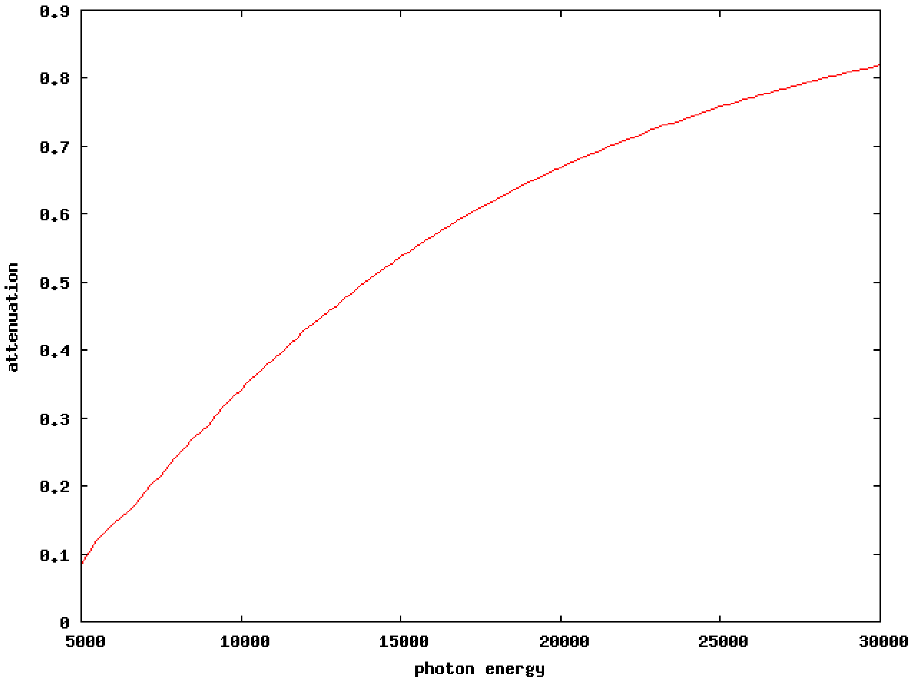
$$2\tau = 21.49 \cdot (\sin(\theta)/\lambda)^{2.45} + 0.61 \tag{8}$$

Calculations – In the previous section the probability to scatter a photon and therefore attenuation due to elastic scattering at one grain with the length l has been calculated. In order to obtain the elastic attenuation of a foil with variable size we think of the foil consisting of many squared grains with the dimensons $l \times l \times l$ (cf. figure 4). The attenuation is given as 1 minus the probability to transit the photon through one grain to the power of the number of grains in the path with length d:

$$\gamma = 1 - (1 - W)^{d/l}. \tag{9}$$

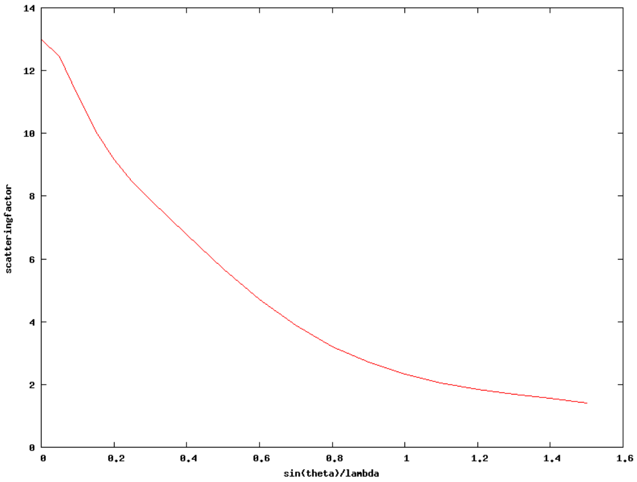
Figure 5 represents calculations done using Java apprications (”dyns.java” and ”bragg.java”)

Figure 5: The attenuation factor γ of a $1mm$ Al foil due to elastic scattering in the "semi" dynamic model. The attenuation increases in with the energy of the photon beam since more planes are accessible to bragg diffraction.



attached in the appendix. The γ calculated for a Al foil with thickness $1mm$ represents solely the attenuation due to the bragg scattering. It turns out that in this calculation the attenuation due to scattering at high energies ($30KeV$) is in the same order like the absorption due to photo ionization ($\gamma \approx 1/10$).

Figure 6: Scattering factor of Al



6.2 Approach via kinematic theory

Thompson scattering – The model for scattering on free electrons can be used in a bound system if the exiting radiations energy is higher than the energy of the absorption edge. This is true for the selected materials and energy ranges in the attenuator-device. The scattering of photon can then be described by a number, which is commonly called the scattering factor f. It expresses the scattering of an atom by scattering on the electron density associated with each atom. In ”International Tables of Crystallography” values for f are calculated using a spherically averaged electron-density distributions. The values therefore only depend on the scattering angle θ as well as on the wavelength λ and is not a complex value.

In the following the derivation of the scattering factor will be retraced and applied to calculate the intensity of elastic scattered photons from a small crystal.

Scattering by a free electron – For a highly polarized beam the amplitude squared of the electric field on the unit sphere ($R = 1$) scattered by a single electron is given by:

$$I = I_0 \frac{e^4}{m^2 c^4} P \tag{10}$$

Where the quantity $\frac{e^4}{m^2c^4} = 7.94 \cdot 10^{-30} m^2$ and P is the polarization factor.

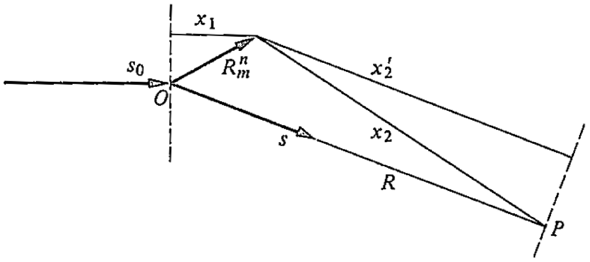
Scattering by an atom – To obtain the amplitude of elastic scattering f from an atom. The scattering of all the electrons n in the shell or their density $\rho(r)$ distribution respectively have to be summed:

$$f = \sum_n \int_0^\infty 4\pi r^2 \rho(r) \frac{\sin(kr)}{kr} dr$$

Herein the abbreviation

$$k = \frac{4\pi \sin(\theta)}{\lambda}$$

Figure 7: Diffraction of a small crystal



represents the spacing in the reciprocal lattice.

As seen in Figure 6 the scattering factor of aluminium decreases with the scattering angle θ from the number of electrons of the shell down to zero. This is due to the coherent scattering of all electrons in the forward direction and the decrease is caused by increasing phase difference with increasing k.

Intensity scattered from a small crystal – To derive the scattered intensity of a small crystal we superposition the scattered intensities of each atom in the crystallites. This is usually called the kinematic approach. Scatterers in the material do not interact with each other and are independent. They are excited by the field in which they are embedded without absorbing energy from this em field. In this sense the kinematic scattering theory is only suitable if the crystals studied contain in the order of $1.2 \cdot 10^{11}$ unit cells. In this derivation we further will utilize the plane wave and the far field approximation, which means that the crystal is far from the source so the wavefront can be considered a plane wave and that the detector is far from the sample which allows further simplification. Figure 7 illustrates the situation. The sample is at position O and the beam is fully polarized normal to the paper. Let $\vec{s}_0$ be the direction of the incident beam, and $\vec{s}$ the direction of the scattered beam, both being unit vectors. The sample is a crystallite which consists of unit cells at the positions $m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3$. The atoms therefore have the position $\vec{R}^m_n = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3 + r_n$. From the figure we see that the difference in length from the initial wavefront to the point of observation is $x_1 + x_2$ which in the far-field approximation becomes $x_1 + x'_2$. Written in terms of the complex exponential the contribution of the atom (m,n) to the field at the detector in P is:

$$\varepsilon_P = \frac{E_0 e^2}{mc^2 R} f_n \exp(2\pi\nu t - (2\pi/\lambda)[\vec{R} - (\vec{s} - \vec{s}_0) \cdot (\vec{R}^m_n)])$$

To receive the total scattered field in the point of the detector we have to sum over all the n atoms in the unit cell and the positions m_1, m_2, m_3 of the unit cells. In the following the shape of the crystal is a parallelepiped with dimensions $N_1 a_1 \times N_2 a_2 \times$

N_3a_3. Considering these conditions equation (11) can be written:

$$\begin{aligned}\varepsilon_P &= \frac{E_0e^2}{mc^2R}\exp(2\pi i(\nu t - R/\lambda))\ F\sum_{m_1=0}^{N_1-1}\exp((2\pi i/\lambda)(\vec{s}-\vec{s_0})\cdot m_1\vec{a_1})) \\ &\times \sum_{m_2=0}^{N_2-1}\exp((2\pi i/\lambda)(\vec{s}-\vec{s_0})\cdot m_2\vec{a_2}))\sum_{m_3=0}^{N_3-1}\exp((2\pi i/\lambda)(\vec{s}-\vec{s_0})\cdot m_3\vec{a_1}))\end{aligned}$$

Herein F is the structure factor of the material. And represent the influence of the atoms in the unit cell on the scattering process.

$$F = \sum_n f_n \exp((2\pi i/\lambda)(\vec{s}-\vec{s_0})\cdot\vec{r}_n)$$

Taking the product $\varepsilon_P\varepsilon_P^*$ multiplied with the polarization factor will give the intensity scattered on the unit sphere ($R = 1$):

$$\begin{aligned}I_P &= I_0P\frac{e^4}{m^2c^4}F^2\frac{\sin^2(\pi/\lambda)(\vec{s}-\vec{s_0})\cdot N_1\vec{a_1}}{\sin^2(\pi/\lambda)(\vec{s}-\vec{s_0})\cdot\vec{a_1}} \\ &\times \frac{\sin^2(\pi/\lambda)(\vec{s}-\vec{s_0})\cdot N_2\vec{a_2}}{\sin^2(\pi/\lambda)(\vec{s}-\vec{s_0})\cdot\vec{a_2}}\frac{\sin^2(\pi/\lambda)(\vec{s}-\vec{s_0})\cdot N_3\vec{a_3}}{\sin^2(\pi/\lambda)(\vec{s}-\vec{s_0})\cdot\vec{a_3}}\end{aligned}$$

Power scattered from a powder sample – The scattered intensity of one grain integrated over the unit sphere (β,γ), over all possible orientations of the grain and over all reflecting planes *hkl* gives the power scattered from the single grain. Summing all grains M in the powder sample yields the scattered power by the sample.

$$IA = \sum_{hkl}\int\int\int I_P\frac{M}{2}\cos(\theta(hkl))d\beta d\gamma$$

The triple integration can be expressed as a volume integration in reciprocal space. It can be show that:

$$IA = I_0\left(\frac{e^4}{m^2c^4}\right)\frac{V\lambda^3F^2}{4v_a^2}P \tag{11}$$

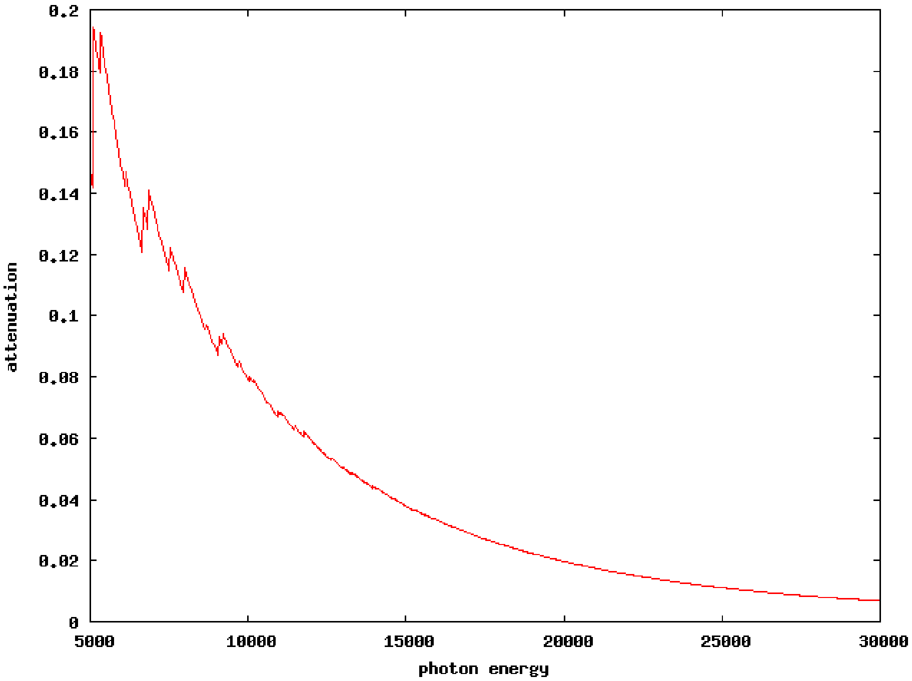
Herein $V = MNv_a$ represents the effective volume of the crystalline material in the powder sample with the volume of the unit cell being v_a and the number of unit cells in a grain being N.

Calculations – With the help of formula (11), found ie. by B.E. Warren in [Warren], the attenuation caused by elastic scattering from a thin metal foil can be calculated. γ is given in dependence of the thickness of the foil l, the wavelength of the radiation λ by:

$$\gamma_{kin} = \sum_{hkl}\left(\frac{e^4}{m^2c^4}\right)\frac{l\lambda^3F^2}{4v_a^2}\frac{1+\cos^2\theta}{2} \tag{12}$$

Which is the sum over all possible (some of which are equivalent) combinations of hkl. The calculations (cf. figure 8) have also been done using Java code (”kins.java” and ”bragg.java”) for a aluminium foil of thickness $1mm$ in the energy range from $5KeV$ to $30KeV$

Figure 8: The attenuation factor γ of a $1mm$ Al foil due to elastic scattering in the kinematic model. The attenuation decreases with the photon energy since the decrease in volume λ^3 dominates over the increase of diffracting planes.



6.3 Comparison of results

The dependence on energy is very different depending on what theory is utilized to obtain attenuation due to elastic scattering.

The approach using the extinction length of a perfect crystal gives a rise of γ with increasing energy possibly to a satuation point or to infinity. The attenuation in the high energy regime also seems unlikely since the calculation predicts that a $1mm$ thin aluminium foil would stop 50% of the photons passing with at an energy of $30KeV$.

The kinematic theory gives a result that approaches zero for high energies but is only applicable for thin foils. This limit of the theoretical approximation to small samples explains why γ_{kin} can be proportional to the thickness of the foil.

$$l \longrightarrow \infty \Rightarrow \gamma_{kin} \longrightarrow \infty \tag{13}$$

The thickness has to be limited otherwise the attenuationr would amplify the beam. On the other hand are the grains of the foils in this size limit which makes this theory probably better suited than the perfect crystal one.

To refine the results of the kinematic approach one could further take temperature effects into consideration. Also subdividing the illuminated material of the foil into smaller parts (cf. principle of figure 4) and calculating the attenuations seperatly would solve the problem with $\gamma \propto l$.

References

[Ash] Ashcroft and Marmin, Solid State Physics, 1976

[Warren] B.E. Warren, X-Ray Diffraction, 1990

[Zac] Zachariasen, Theory of X-Ray Diffraction in Crystals, 1967

[Lau] Max von Laue, Röntgenstrahlinterferenzen, 1941

A Charts

A.1 Scattering factor

Atomic Scattering Factors*

$(\sin\theta)/\lambda(A^{-1})$		0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
H	1	1.0	0.81	0.48	0.25	0.13	0.07	0.04	0.02	0.02	0.01	0.01					
He	2	2.0	1.83	1.45	1.06	0.74	0.52	0.36	0.25	0.18	0.13	0.10	0.07	0.05	0.04	0.03	0.03
Li	3	3.0	2.22	1.74	1.51	1.27	1.03	0.82	0.65	0.51	0.40	0.32	0.26	0.21	0.16		
Be	4	4.0	3.07	2.07	1.71	1.53	1.37	1.20	1.03	0.88	0.74	0.62	0.52	0.43	0.37		
B	5	5.0	4.07	2.71	1.99	1.69	1.53	1.41	1.28	1.15	1.02	0.90	0.78	0.68	0.60		
C	6	6.0	5.13	3.58	2.50	1.95	1.69	1.54	1.43	1.32	1.22	1.11	1.01	0.91	0.82	0.74	0.66
N	7	7.0	6.20	4.60	3.24	2.40	1.94	1.70	1.55	1.44	1.35	1.26	1.18	1.08	1.01		
O	8	8.0	7.25	5.63	4.09	3.01	2.34	1.94	1.71	1.57	1.46	1.37	1.30	1.22	1.14		
F	9	9.0	8.29	6.69	5.04	3.76	2.88	2.31	1.96	1.74	1.59	1.48	1.40	1.32	1.25		
Ne	10	10.0	9.36	7.82	6.09	4.62	3.54	2.79	2.30	1.98	1.76	1.61	1.50	1.42	1.35	1.28	1.22
Na	11	11.0	9.76	8.34	6.89	5.47	4.29	3.40	2.76	2.31	2.00	1.78	1.63	1.52	1.44	1.37	1.31
Na^+	11	10.0	9.55	8.39	6.93	5.51	4.33	3.42	2.77	2.31	2.00	1.79	1.63	1.52	1.44	1.37	1.30
Mg	12	12.0	10.50	8.75	7.46	6.20	5.01	4.06	3.30	2.72	2.30	2.01	1.81	1.65	1.54		
Al	13	13.0	11.23	9.16	7.88	6.77	5.69	4.71	3.88	3.21	2.71	2.32	2.05	1.83	1.69	1.57	1.48
Si	14	14.0	12.16	9.67	8.22	7.20	6.24	5.31	4.47	3.75	3.16	2.69	2.35	2.07	1.87	1.71	1.60
P	15	15.0	13.17	10.34	8.59	7.54	6.67	5.83	5.02	4.28	3.64	3.11	2.69	2.35	2.10	1.89	1.75
S	16	16.0	14.33	11.21	8.99	7.83	7.05	6.31	5.56	4.82	4.15	3.56	3.07	2.66	2.34		
Cl	17	17.0	15.33	12.00	9.44	8.07	7.29	6.64	5.96	5.27	4.60	4.00	3.47	3.02	2.65		
Cl^-	17	18.0	16.02	12.20	9.40	8.03	7.28	6.64	5.97	5.27	4.61	4.00	3.47	3.03	2.65	2.35	2.11
A	18	18.0	16.30	12.93	10.20	8.54	7.56	6.86	6.23	5.61	5.01	4.43	3.90	3.43	3.03		
K	19	19.0	16.73	13.73	10.97	9.05	7.87	7.11	6.51	5.95	5.39	4.84	4.32	3.83	3.40	3.01	2.71
Ca	20	20.0	17.33	14.32	11.71	9.64	8.26	7.38	6.75	6.21	5.70	5.19	4.69	4.21	3.77	3.37	3.03

(*cont.*)

* Reprinted from *International Tables for X-Ray Crystallography*, Vol. III, with the permission of the Editorial Commission of the International Tables. The values for elements 1–36 are computed from self-consistent or variational wave functions, while those for elements 37–92 are obtained from the Thomas-Fermi-Dirac statistical model. For values corresponding to ionized states, reference should be made to the International Tables.

B Code

B.1 bragg.java

```
import java.util.*;
import java.math.*;
import java.io.*;

public class bragg{
    static double a = 4.049e-10;
    static double h = 6.62606896e-34;
    static double e = 1.602176487e-19;
    static double c = 2.99792458e8;

    public static double getLambda(double energy){
        return(h*c/(energy*e));
    }

    public static double distance(int h, int k, int l){
        return(Math.sqrt(a*a/(h*h+k*k+l*l)));
    }

    public static int geometricStructureFactor(int h, int k, int l){
        return((int)(1+ Math.pow(-1,h+k) + Math.pow(-1,k+l) + Math.pow(-1,l+h)));
    }

    public static double angle(int h, int k, int l, double lambda){
        return(Math.asin(lambda/(2*distance(h, k ,l))));
    }

    public static double polarisation(double theta){
        return((1+Math.pow(Math.cos(theta),2))/2);
    }

    public static Vector planes(double energy){
        int h,k,l;
        double lambda = getLambda(energy);
        Vector planesAdv = new Vector();
        Vector planes = new Vector();
        h=0;
        while((2*distance(h,k=0,l=0))>lambda){
            k=0;
            while((2*distance(h,k,l=0))>lambda){
                l=0;
                while((2*distance(h,k,l))>lambda) planes.add(new int[]
                    {Math.abs(h),Math.abs(k),Math.abs(l++)});
                l=-1;
                while((2*distance(h,k,l))>lambda) planes.add(new int[]
                    {Math.abs(h),Math.abs(k),Math.abs(l--)});
            k++;
            }
            k=-1;
            while((2*distance(h,k,l=0))>lambda){
                l=0;
                while((2*distance(h,k,l))>lambda) planes.add(new int[]
                    {Math.abs(h),Math.abs(k),Math.abs(l++)});
                l=-1;
```

```
                while((2*distance(h,k,l))>lambda) planes.add(new int[]
                    {Math.abs(h),Math.abs(k),Math.abs(l--)});
            k--;
            }
        h++;
        }
        h=-1;
        while((2*distance(h,k=0,l=0))>lambda){
            k=0;
            while((2*distance(h,k,l=0))>lambda){
                l=0;
                while((2*distance(h,k,l))>lambda) planes.add(new int[]
                    {Math.abs(h),Math.abs(k),Math.abs(l++)});
                l=-1;
                while((2*distance(h,k,l))>lambda) planes.add(new int[]
                    {Math.abs(h),Math.abs(k),Math.abs(l--)});
            k++;
            }
            k=-1;
            while((2*distance(h,k,l=0))>lambda){
                l=0;
                while((2*distance(h,k,l))>lambda) planes.add(new int[]
                    {Math.abs(h),Math.abs(k),Math.abs(l++)});
                l=-1;
                while((2*distance(h,k,l))>lambda) planes.add(new int[]
                    {Math.abs(h),Math.abs(k),Math.abs(l--)});
            k--;
            }
        h--;
        }
        planes.removeElementAt(0);
        for (int i = 0; i<planes.size(); i++){
            int[] plane = (int[]) planes.get(i);
            if(((int)geometricStructureFactor(plane[0],plane[1],plane[2]))==0) {
                    planes.removeElementAt(i);
                    i--;
            }
        }
        return(planes);
    }
}
```

B.2 kins.java

```java
import java.util.*;
import java.math.*;
import java.io.*;

public class kins{
    static double cer = 2.8178e-15; //m
    static double v = Math.pow(bragg.a,3);

    public static double F(int h, int k, int l){
        return(scatteringFactor(h, k, l)*bragg.geometricStructureFactor(h, k, l));
    }

    public static double scatteringFactor(int h, int k, int l){
        return(13.1319*Math.exp(-1.68985/(2e10*bragg.distance(h, k, l))));
    }

    public static double scatteredIntensity(double energy , double thickness){
        double lambda = bragg.getLambda(energy);
        Vector planes = bragg.planes(energy);
        int size = planes.size();
        double R = 0;
        double lambda3 = Math.pow(lambda,3);
        double cer2 = Math.pow(cer,2);
        double v2 = Math.pow(v,-2);
        for(int i=0; i<size; i++){
            int[] plane = (int[]) planes.get(i);
            double F2 = Math.pow(F(plane[0],plane[1],plane[2]),2);
            double P = bragg.polarisation(bragg.angle(plane[0],plane[1],plane[2], lambda));
            R = R + cer2 * thickness * lambda3 * F2 * 0.25 * v2 * P;
        }
        return(R);
    }

    public static void main(String[] A) throws Exception{
        FileWriter out = new FileWriter("kinout.dat");
        double energy;
        for(int i=0; i<101; i++){
            energy = ((double) i)*25000/100 + 25000;
            out.write(((i*5000/100)+5000) + "\t" + scatteredIntensity(energy,1e-3) + "\n");
        }
        out.close();
    }
}
```

B.3 dyns.java

```java
import java.util.*;
import java.math.*;
import java.io.*;

public class dyns{
    static double delta = 1.75e-5;

    public static double probOrientation(double theta){
        return((delta/2)*Math.cos(theta));
    }

    public static double dynamicExtinction(int h, int k, int l, double length){
        double sl = 1/(2*bragg.distance(h,k,l)*1e10);
        double a = 21.49;
        double b = 2.45;
        double c = 0.61;
        double L = a*Math.pow(sl,b)+c;
        return(1-(Math.exp(- length * 1e6 / (L/2)) ));
    }

    public static double photoT(double energy, double length) throws Exception{
        return(Math.exp(-(length*1e6/attenuation.getLambda(energy, "Al"))));
    }

    public static double scatteredIntensity(double energy, double thickness, double length){
        double lambda = bragg.getLambda(energy);
        Vector planes = bragg.planes(energy);
        int size = planes.size();
        double R = 0;
        for(int i=0; i<size; i++){
            int[] plane = (int[]) planes.get(i);
            double theta = bragg.angle(plane[0],plane[1],plane[2],lambda);
            R = R + probOrientation(theta) * bragg.polarisation(theta) *
                dynamicExtinction(plane[0],plane[1],plane[2], length);
        }
        double T = 1-R;
        return(1-Math.pow(T,(thickness/length)));
    }

    public static void main(String[] A) throws Exception{
        FileWriter out = new FileWriter("dynout.dat");
        double energy;
        for(int i=0; i<101; i++){
            energy = ((double) i)*25000/100 + 5000;
            out.write(((i*25000/100)+5000) + "\t" + scatteredIntensity(energy,1e-3,1e-6) + "\n");
        }
        out.close();
    }
}
```