

# [A novel technique for x ray spectroscopy environmental sciences essay](https://assignbuster.com/a-novel-technique-for-x-ray-spectroscopy-environmental-sciences-essay/)

By utilising different Ross filter pairs, each with a different discrete pass band, the low energy X-ray spectrum becomes observable. This is the aim of the chapter; to determine a set of Ross filter pairs that provide high spectral resolution and a high transmittance to observe the X-ray energy range of 10 KeV - 100 KeV. A compromise will have to be reached between these aims and choosing a practical number of safe, commercially available and non-radioactive materials to be implemented as the Ross filters. The K-edges that arise due to photoelectric absorption are well defined and are unique to each element, and the energy at which they occur is at higher energies for high Z elements and at lower energies for low Z elements. It is the K-edges that were utilised by P. A. Ross to define the limits of the Ross filter pass bands. In this section, the method for creating Ross filter pairs with defined energy limits is explained, based on utilising the Beer-Lambert law to model the transmittance of radiation through the filter material. The transmission curve for each material at different thicknesses is calculated by the normalised Beer-Lambert law, using density values and X-ray attenuation coefficients for each element obtained from a database provided by the National Institute of Standards and Technology [NIST]. The transmission curves and the Ross filter pass bands are plotted using Microsoft Excel 2010. Two filters are placed side by side in an X-ray beam and the transmission of the radiation through each is recorded. The thicknesses of the filters are adjusted so that the transmission curves of each are identical, apart from the regions defined by the characteristic K-edge of each. For example, Figure [fig: ZnTiMA] shows the transmission curves for zinc and titanium filters. The filter thicknesses are adjusted to obey the above criteria and the difference in transmission within the K-edge region is clearly visible. By electronically subtracting the high Z filter transmission curve from the low Z filter transmission curve, all that is left is a pass band due to the transmittance difference between the K-edges as shown by the example in Figure [fig: ZnTiRF]. The filters produce a monochromatising effect [KP\_RF1] allowing for the Beer-Lambert law to be utilised. This is the technique developed by Ross, and it has been utilised to create Ross filter based spectrometers in a variety of experimental settings. One of the more recent examples includes the use of Ross filters to characterise X-ray sources during Inertial Confinement Fusion (ICF) experiments at the National Ignition Facility in California [NIF2] , where the electromagnetic pulse generated by the laser-matter interaction makes finding a diagnostic capable of withstanding it challenging [Maddox 2011]. This is the method on which the design of the Ross filters for the first diagnostic component will be determined. However, as can be seen in Figure [fig: ZnTiRF], even though a well defined pass band is created, there exists regions either side of the pass band of unwanted spectral sensitivity. This is due to the filters not being perfectly matched. Obtaining a " perfect match" is not possible because attenuation is dependent on the Z number of the materials used and different materials have to be used to create a discrepancy between the K-edges. The seemingly negative transmission outside the low energy limit is due to the low Z filter transmitting more radiation than the high Z filter across that particular energy range. To achieve the best possible matching, filters consisting of elements with adjacent atomic numbers should be utilised, since they have the most similar transmission curves to one another (as they have the most similar amount of protons to one another). This would also provide the best spectral resolution, as the K-edges of each would be very similar, hence narrower pass bands would be obtained. However, this is impractical for a number of reasons. Firstly, the energy range this diagnostic component operates across is from 1 - 100 KeV, meaning that every element between aluminium and uranium (K-edge values of 4. 96 KeV and 115. 6 KeV respectively [NIST]) would have to be used to construct an enormous amount of Ross filter pairs. This conflicts with the aims of this project to design a cheap and compact diagnostic and it is clearly unfeasible to consider. Secondly, hazardous, radioactive and rapidly oxidising materials would have to be used which is undesirable. As such, an alternative method must be considered to reduce the amount of unwanted transmission. In 1994, I. Khutoretsky developed a novel method for reducing the response of Ross filters outside of the desired sensitivity range [Khutoretsky] by adding an even lower Z element to the low Z filter. Khutoretsky used aluminium as the additional element since it has a low density, is readily available and is safe and reusable [Al]. Figure [fig: TiAlZnRF] shows the result of adding aluminium to the titanium filter of the Ross filter pair shown in Figure [fig: ZnTiRF]. The thickness of the titanium filter is adjusted to accommodate for the extra aluminium. A large reduction in the amount of unwanted transmission is observed, especially before the filter pair's low energy limit. The filter pair's sensitivity past the high energy limit is still present, but it has been reduced. However, in this particular case the shape of the pass band becomes more non-uniform as a result of adding the aluminium. The highest energy K-edge that can be utilised to create Ross filter pass bands is that of uranium's, which occurs at 115. 6 KeV. However, uranium is a highly undesirable material due to its radioactivity, as are all of the actinides; the elements that have K-edges at the highest energies. As such, in reality the high energy limit that Ross filters can be utilised up to is that of lead, at 88 KeV [NIST]. To observe X-rays that have a higher energy than this is not possible by using Ross filters designed using the conventional method. An alternative method has been proposed by R. Clarke (Central Laser Facility, Rutherford Appleton Laboratory). Instead of adjusting the thickness of each filter to match the K-edges, the K-edge of the high Z filter is matched to the transmission curve of the low Z filter. Figure [fig: TiZnMAN] illustrates this technique for a Ti-Zn filter pair. The K-edge of Zn is matched to the transmission curve of Ti, and then by subtracting the Zn transmission curve from the Ti transmission curve, the pass band shown in Figure [fig: TiZnRFN] is obtained. This technique allows for a higher energy pass band to be obtained from a particular Ross filter pair than is possible with the conventional method. The main advantage of this is that energies higher than the K-edge of Pb are now possible to be observed by Ross filters, without the need for any actinides. The disadvantages of this technique are made clear by the figures below. The pass band itself has a very wide energy range, meaning that only low resolution would be obtainable if this technique was used to model the entire energy range from 1 - 100 KeV. There is also the issue of undesirable sensitivity due to the unmatched K-edge of the the low Z filter. It is possible to reduce this effect by using a low Z filter with a high thickness so that there is too much attenuation for the K-edge to be visible. However, this would have to be balanced with the requirement for good matching between the filters, as increasing the thickness of a filter will also alter shape of the transmission curve as well as the K-edge. In this section, the criteria for elements that would be ideal to be used as filters are outlined based upon the mass attenuation coefficient and the physical properties of the element. The statistical technique of linear interpolation is explained and it's crucial role in modelling the pass bands is justified. The pass bands are then modelled using a combination of the three matching techniques to cover the energy range of 1 KeV - 100 KeV and to obtain the best resolution possible. An attempt to reduce the number of Ross filters needed to model the desired energy range is presented, and conclusions are drawn to determine the final configuration of pairs to make up the filter wheel. To produce a Ross filter wheel that covers the desired energy range in 10 KeV increments, it would be ideal to utilise materials that have K-edges in approximately 10 KeV increments since it is the K-edges that define the limits of the pass band. However, there are materials that are unsuitable for use. Materials that are difficult to manufacture into very thin foils and those of which are expensive and rare will be omitted. Materials that are radioactive or hazardous, that readily oxidise or are reactive with water are also omitted. This set of criteria limits the choices of materials suitable for use to the metals. Metals are readily available and are easily processed into thin foils. However, they do not cover all of the desired energy range, in particular the energy range between 30 KeV - 70 KeV. The elements that have K-edges within this energy range are known as lanthanides, and most of them readily oxidise (thus altering their attenuation coefficient) or are radioactive. The choice of metals to be utilised as Ross filters is determined by both the energy at which their K-edges occur and their physical properties. Information on the properties of various metals was obtained from their entries in C. Hampel's " The Encyclopedia of the Chemical Elements" respectively [Elements]. Finally, to ensure maximum transmission through a filter, a low thickness must be used. However, this is limited by how thin the filters can be manufactured. Filters which are very thin would be easily damaged by being handled and mounted into place. If there were a rip or a hole in the filter then unwanted radiation would leak through, resulting in inaccurate and unreliable data. Thin filters could also be bent and deformed easily, altering the effective thickness of the filter and again making the obtained data unreliable. As such, a limit on how thin the filters can be is set at 10 microns; a thickness that can be manufactured quite easily in material fabrication laboratories (in fact, the Target Fabrication Facility at the CLF can manufacture foils less than 100nm thick [TargetFab]). The data used to model the Ross filter pass bands is obtained from the NIST website. For example, abstracts of the data sets for titanium and zinc are shown in Figure [fig: TiZnTable]. The table shows how the mass attenuation coefficient of each element varies depending on the energy of the incident radiation. To create a pass band using these two materials, the energy dependent mass attenuation coefficients of Ti are subtracted from those of Zn. However, as can be seen in the figure, the energy data points are different and so the data points do not match. This is due to there being extra data points around the absorption edges of each element. These extra data points exist to accurately map the sudden jump in the mass attenuation coefficient over a infinitesimally small energy range. Simply put, the resultant subtraction would be incorrect since the data sets do not contain the same energy data points. To remedy this, linear interpolation is implemented to estimate the extra data points in each data set so that they can be correctly subtracted. Over a small range of data, the relationship between each point can be assumed to be linear. The equation for linear interpolation between two points is: where y= mass attenuation coefficient and x= energy. This process is an approximation, and as such will inherently result in error which will need to be accounted for. Figure [fig: TiZnTableLin] shows the result of implementing linear interpolation on the data set in Figure [fig: TiZnTable]. The data points now match up and they can be subtracted to produce the correct pass band for the two filters. To model a Ross filter pair, Excel is utilised to determine the transmission curve for each filter within the pair by using the Beer Lambert law, density and X-ray attenuation data for that particular element and linear interpolation to fill in the gaps within the data sets. The spreadsheets of data along with transmission curves and pass bands plotted are many and so have all been included on the CD that accompanies this report. Information on how to understand the tables is contained within Appendix 1. The method for how the pass band for each Ross filter was modelled is as follows:• Two metals were chosen based on what energy their K-edges occur at to form the limits of the pass band.• The physical properties of the chosen materials were checked to make sure they obeyed the set criteria. If they did not, then another material with a similar K-edge was chosen instead.• X-ray attenuation data for each metal is tabulated into Excel.• The Beer-Lambert law is used to create the transmission curves of each filter.• Linear interpolation is implemented to match the data sets.• The thicknesses of each are adjusted to match the K-edges of each transmission curve.• The transmission curve of the low Z filter is subtracted from that of the high Z filter to produce the pass band.• The thicknesses are again adjusted to optimise the pass band; ie. to maximise the peak transmission whilst reducing the response outside of the sensitivity range. To start with, the only limitation placed on the design of each Ross filter pair is that the thickness of each filter must be greater than 10 microns. Not restricting which materials can be used allows an " ideal" Ross filter spectrum to be modelled; one which has the high resolution outlined in the project aims. Following the methodology and by implementing the conventional method of matching the K-edges, the Ross filter pairs were determined and are presented in Figure [fig: RF1\_Table]. Figure [fig: Ideal-Ross-filter] presents the pass bands obtained from this selection of Ross filters. As can be seen from the figure, the limits of each pass band are extremely well defined as expected from the theory. The metal used as the high Z filter of one Ross filter is used as the low Z filter of the next Ross filter. This means that there are no gaps within the spectrum, since the same K-edge is used to define the boundary between each pass band. As long as the pass band is well defined, the Ross filter will not observe any radiation observed by another. However, as can be seen by Figure [fig: Ideal-Ross-filter], there are regions of sensitivity outside of the pass bands for each Ross filter. This is to be expected since it is not possible to perfectly match the transmission curves of two materials with different Z numbers [Soules]. As such, regions of unwanted sensitivity are more difficult to minimise when the size of the pass band is increased. This is because a larger pass band means that there is a greater discrepancy between the K-edges of the two filters used, and so there is a greater difference between the transmission curves as a whole. The peak transmission of each pass band decreases as the energy of the incident radiation increases. This is to be expected from attenuation theory; it takes a thicker high Z filter to effectively attenuate high energy radiation as implied by Eqn ([eq: Absorption]). As a consolation, the increased attenuation of higher energy X-rays further protects the electronic equipment and detectors from damage. In retrospect, as long as we know the transmittance of each pass band, then the amount of photons observed within a given pass band can be multiplied by the transmittance to obtain the true amount of photons emitted by the plasma in the direction of the diagnostic. Transmission outside of the pass bands remains a source of error. To minimise this error, Khutoretsky's method of adding aluminium to the low Z filter of a pair is implemented. This is achieved by using the methodology with the following alterations:• To model the low Z filter with added aluminium, Eqn ([eq: Compound]) must be implemented since the filter is now a compound. Both the chosen material and aluminium have different mass attenuation coefficients, so the amount of each present in the filter must be accounted for.• This is carried out by determining the weight fractions of each element present in the filter, which in this case is equal to the thickness of the element divided by the thickness of the filter as a whole.• Once the weighted mass attenuation coefficients have been determined, the addition of the two provides the total mass attenuation coefficient for the filter. This is then used with the total thickness of the filter in the Beer-Lambert Law to provide the transmission curve.• Linear interpolation must again be implemented to match up the material to the aluminium, which must then be matched to the data set for the high Z material. The same Ross filter pairs used in Section [sub: RFs] are modified to incorporate Khutoretsky's method. The thicknesses for each filter is presented in Figure [fig: RF1\_Al\_Table], and the pass bands are presented in Figure [fig: Ideal-Ross-filter-Al]. As can be seen in the figure, the sensitivity outside of the desired pass bands has been reduced, particularly at low X-ray energies. This is because low energy X-rays are more easily attenuated due by photoelectric absorption than high energy X-rays. In the original paper by Khutoretsky, the sensitivity outside of the pass bands constructed is reduced by more than 5 times [Khutoretsky]. As shown above, a similar reduction is obtained. There is an even greater decrease outside of the low energy pass bands. This is because the low Z filters that are used to attenuate low energy X-rays have a similar Z number to that of aluminium, allowing for a more accurate matching of transmission curves. This results in the increased attenuation of unwanted radiation for a given pass band. The effects of adding aluminium across higher energy pass bands is still visible but less pronounced, again owing to the difference in Z-numbers between the filters and aluminium. This poses the question of whether using a higher Z additional filter instead of aluminium would result in a larger decrease of unwanted sensitivity across higher X-ray energies; this is a possible avenue of future work. Even though the Ross filter spectra already modelled achieve the aim of high spectral resolution by using 10 keV wide pass bands, undesirable materials are used. All of the ideal material criteria are now implemented, meaning that all materials that readily oxidise or are radioactive are omitted; ie. the lanthanides and the actinides. This will result in a 40 KeV pass band covering 30 KeV-70 KeV, diminishing the spectral resolution. Upon research into the properties of all the lanthanides, gadolinium has proven an ideal candidate for use since it does not readily oxidise, it's malleable and easy to work and it not hazardous to health unless ingested. The K-edge of gadolinium occurs at approximately 50 KeV [Gadolinium K] and so the energy range of 30 KeV-70 KeV can be observed by two 20 KeV wide pass bands. To observe the energy range covered by the (Pb, Th) Ross filter, R. Clarke's method is implemented by using a (Ti, Pb) Ross filter. The thicknesses for each filter are presented in Figure [fig: Ross-filter-pairs, NM], and the resultant pass bands are presented in Figure [fig: Optimal-Ross-filter]. With no undesirable materials used, the pass bands remain well defined and a good spectral resolution is maintained. However, the energy range covered by the final pass band is elongated by a large " tail," an issue which is unfortunately unavoidable when implementing the novel method. This is because a K-edge isn't utilised to provide the high energy limit of the pass band. Such a large tail will result in a large amount of error in the data measurements across this energy range. One way to possibly reduce this error is to instead define the limits of the pass bands by the Full Width Half Maximum (FWHM); a parameter used to define curves by what their width is at half of their maximum value [FWHM]. This is a parameter commonly implemented in determining the pass bands of optical filters [Edmund] that operate in other regions of the EM spectrum where the pass bands aren't so well defined. If the highest energy pass band is defined in this way, then it is approximately covers 88 KeV - 125 KeV, but a large tail still remains. So far, the aim of providing high spectral resolution has been achieved. However, sixteen different filters are used to construct the eight Ross filters and even though the dimensions of the filters do not have to be very large (for example, they could be the same size or smaller than the detectors behind them) the design could be more compact. A variation in the construction of Ross filters was implemented by David J. Johnson in 1973. Instead of using a pair of different materials to construct each Ross filter, triplet sets of filters were used [Johnson]. In other words, one particular filter acts as both the high Z filter of one Ross filter and the low Z filter of the next, so three filters instead of four filters construct two pass bands The disadvantage of this method is that the thickness chosen for the particular filter may match well for one Ross filter, but it may not for the other. By implementing this method, the thicknesses for the filters chosen are presented in Figure [fig: Ross-filter-triplet] and the resultant pass bands are presented in Figure [fig: Ross-filter-triplets\_spec]. The same energy range is observed by eight pass bands, but only twelve filters are needed to construct them instead of sixteen. Due to the problems with matching a material with the same thickness to both a material of lower and higher Z, the quality of the pass bands is diminished. Aluminium cannot be added to the low Z filters that are also used as the high Z filters of another pass band, resulting in increased sensitivity outside of the pass bands. This is especially evident for the Sn-Gd Ross filter, where the L-edge of Gd is visible. In all of the other spectra modelled the high Z filters are thick enough so that L and M absorption edges are minimised. In the modelling of the Ross filters, the only uncertainty that can be taken into account is that of the density and mass attenuation coefficients of the materials utilised. The data sets on the NIST website are determined from two different data bases; XCOM and FFAST [XCOM-FFAST1]. The attenuation coefficients are determined from theoretical calculations and approximations, and as such will inherently carry uncertainty. The transmission outside of the pass bands also provides uncertainty in the measurements. Determination of the uncertainty due to these " tails" is considered an area of future work. In practical terms, one of the main sources of error would be how accurately the filter thicknesses can be manufactured. As shown from the theory, even a small change such as a few microns in thickness of one filter can unmatch the Ross filter and cause unwanted transmission outside of the pass band. The filters would also have to be mounted as parallel as possible to each other so that the effective thickness of each is the same (since if the photon entered a filter placed at an angle then the filter would appear thicker than it actually is). Even though photoelectric absorption is the dominant attenuation factor across the observed energy range, background radiation due to Compton scattering is to be expected since the filters provide scattering targets. In this chapter, various methods used to determine Ross filter pass bands have been discussed based on attenuation theory. These methods have been implemented with the project aims and a set criteria in mind, and steps were taken to improve the modelled pass bands. An attempt to reduce the amount of filters needed was also presented, and comparisons were drawn between the Ross filters modelled and those utilised in experiments previously. Taking all of this into consideration, the Ross filter data presented in Figures [fig: Ross-filter-pairs, NM] and [fig: Optimal-Ross-filter] will be utilised in the final design of the diagnostic. This choice of Ross filters satisfies all of the set criteria. Even though it is not as compact as the set-up in Figure [fig: Ross-filter-triplets\_spec], the pass bands are more uniform and there is less transmission outside of the pass bands. These factors outweigh the option to reduce the number of filters from sixteen to twelve.