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Controlling Dose to Low Z Solids at LCLS

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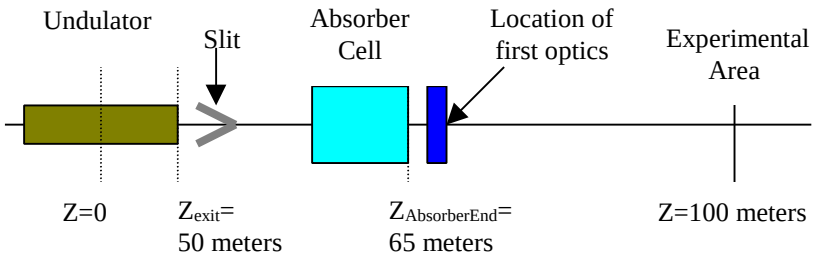
Abstract

Calculations of the dose suffered by the low Z solids, Li, Be, B, B_4C, BeO and C at various points along the Linac Coherent Light Source (LCLS) beam line as a function of FEL photon energy are presented. Specific column densities of attenuator gases necessary to control the dose to C are calculated for assumed damage thresholds of 0.1 eV/atom and 0.01 eV/atom.

Introduction

Although the average power delivered by the LCLS is modest, there is great concern that the short, intense, FEL pulse will damage materials placed in the beam. These concerns impact both safety considerations and optics design.

The LCLS facility includes a gas absorber upstream of the users to attenuate the beam as shown in the figure.



- Figure 1: Layout of LCLS FEL beam line areas.

As shown, the most upstream position for any x-ray optics would be just downstream of the absorber. The most likely materials for x-ray optics at this position are mixtures of the low Z solids, Li, Be, B, C, Na, Mn, Al, and Si. Dose calculations at the absorber exit position presented below show that it will be easy to damage any of these materials at the LCLS. In particular, these calculations indicate that Na, Mn, Al, and Si will be damaged at *all* FEL energies. And depending on the exact damage threshold, each of the remaining low Z solids will suffer damage for FEL settings below a certain energy.

To prevent damage the absorption cell must be filled with a gas at sufficient density to lower the intensity below the damage threshold of the beam line optics at the desired FEL wavelength. As a precautionary measure, one may want to *always* require a minimal amount of attenuator gas sufficient to protect the beam line optics at all possible FEL wavelengths. Since the choices of gas are limited, it is of practical importance to calculate the minimal gas densities necessary to assure survival of the low Z solids, both at particular FEL wavelengths, and at all FEL wavelengths.

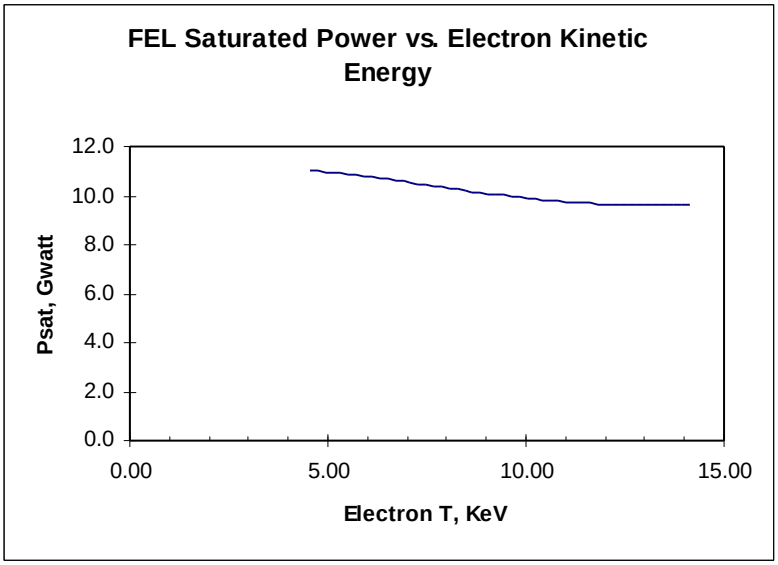
Once the intensity is lowered enough to assure survival of a particular low Z element, blocks of it may be used to provide attenuation for higher Z elements. I have chosen C as an example of a practical low Z sold in the calculations below, and have calculated for each FEL wavelength the density of each candidate gas needed to prevent damage to C at that particular wavelength. I have also calculated a fixed, "safe", density for each candidate gas that will prevent damage to C no matter what the wavelength setting.

The probability of ionizing a single atom in the photon beam is $r_{photon} \cdot s_{photoion}$ where $s_{photoion}$ is the wavelength-dependent atomic photo ionization cross section and r_{photon} is the number of photons per unit area at the position of the atom. Assuming that upon absorption the entire photon energy, E_{photon}, is distributed amongst all the atoms in the material, the average dose to a single atom is: $\overline{Dose} = E_{photon} \cdot r_{photon} \cdot s_{photoion}$.

The atomic photo ionization cross sections are obtained from the Henke tables[i]; the photon density at the absorber exit must be calculated from the expected FEL saturated power levels by propagating a Gaussian beam of the appropriate amplitude from its origin within the undulator to the position of the absorber exit.

FEL power and spatial distribution

The FEL saturated power levels, P_{sat}, and fundamental photon energy, E_{photon}, were calculated vs. electron kinetic energy, T, using the formalism outlined in the LCLS Design Study[ii]. Figure 2 shows the result.



- Figure 2: LCLS expected FEL saturated power level.

Given the saturated power levels, the number of photons per pulse is $N_{photon} = \frac{P_{sat} \cdot t_{bunch}}{E_{photon}}$ with $t_{bunch} = 233 \cdot femtosecond$ defined to be the length of the pulse.

The FEL pulse is modeled as a Gaussian beam that has a plane phase front at the plane $z = z_0$ inside the undulator. The FEL electric field amplitude during the pulse, at a downstream position (x, y, z), is then

$$E(x,y,z,t) = e^{i\cdot wt\cdot t}\cdot e^{-i\cdot k\cdot(z-z_0)}\cdot\frac{p\cdot w_0^2\cdot k}{-w_0^2\cdot k+2\cdot i\cdot(z-z_0)}\cdot e^{\left(-\frac{x^2+y^2}{w(z-z_0)^2}\right)}\cdot e^{\left(-\frac{1}{2}\cdot\frac{i\cdot k\cdot(x^2+y^2)}{R_c(z-z_0)}\right)}$$

The Gaussian waist and phase curvature are functions of the distance from z_0:

$$w(z-z_0)^2 = \frac{(z-z_0)^2\cdot l^2}{p^2\cdot w_0^2} + w_0^2$$

$$R_c(z-z_0) = (z-z_0) + \frac{1}{4}\cdot\frac{w_0^4\cdot k^2}{(z-z_0)}.$$

The parameter w_0 is the 2 dimensional RMS radius of the electric field amplitude at $z = z_0$, where the distribution is narrowest. It is assumed that the electric field amplitude at $z = z_0$ matches the spatial distribution of the electron beam in the undulator.

The spatial distribution of the electron beam is a Gaussian of the form:

$$r_{electron} = \frac{N_{electron}}{2\cdot p\cdot s_e^2}\cdot e^{-\frac{1}{2}\cdot\frac{(x^2+y^2)}{s_e^2}}$$

with s_e varying between 36.2 microns at an electron kinetic energy of $T_{min} = 4.54\cdot GeV$ to 30.5 microns at $T_{max} = 14.35\cdot GeV$. The assumption that the electric field amplitude and the transverse electron beam distributions overlap at $z = z_0$ implies that $w_0 = \sqrt{2}\cdot s_e$.

The plane $z = z_0$ is assumed to be 1 Rayleigh length, $L_R(l) = \frac{2\cdot p\cdot s_e^2}{l}$, from the exit of the undulator: $z_0 = z_{exit} - L_R(l)$. In the coordinate system whose origin at $z = 0$ is at the center of the undulator, the undulator exit is at $z_{exit} = 50\cdot meters$.

The electric field intensity at a given z integrated over the duration of the pulse is:

$$|E|^2\cdot t_{bunch} = |p|^2\cdot t_{bunch}\cdot\frac{w_0^2}{w(z-z_0)^2}\cdot e^{-2\cdot\left(\frac{x^2+y^2}{w(z-z_0)^2}\right)}.$$

The density of photons passing through the plane z is proportional to the electric field intensity so the photon density is of the form:

$$r_{photon}(x,y,z) = A_{peak}(z)\cdot e^{\left(-2\cdot\frac{x^2+y^2}{w(z-z_0)^2}\right)}.$$

$A_{peak}(z)$, the peak photon density at $x = y = 0$, is obtained by setting the integral over the transverse coordinates equal to the total number of photons. The result is:

$$A_{peak}(z) = \frac{2\cdot N_{photon}}{p\cdot w(z-z_0)^2}.$$

This peak photon density is the relevant parameter in the dose calculations.

The beam parameters at the absorber exit for the minimum and maximum electron kinetic energies are summarized in the following table:

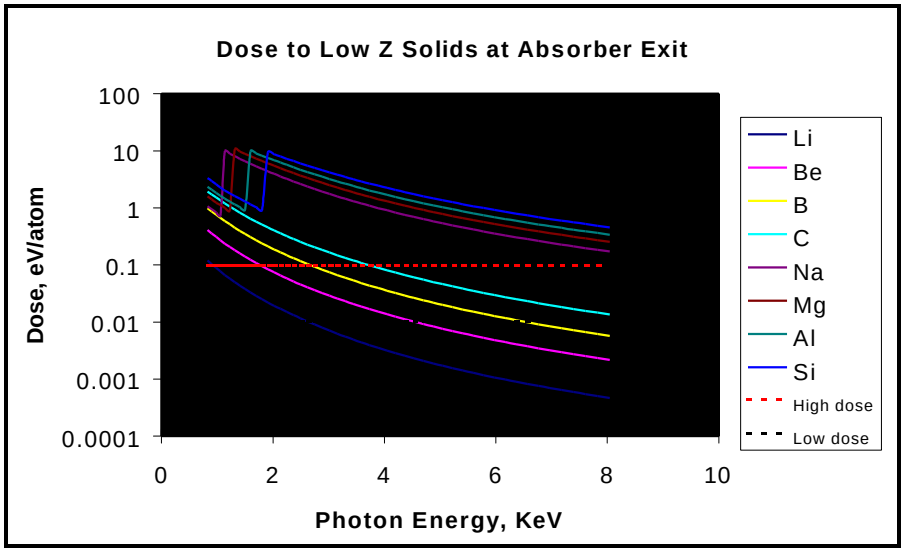
• Table 1: FEL parameters at absorber exit.

	Minimum	Maximum	Units
Electron kinetic energy, T	4.54	14.35	GeV
Fundamental wavelength, l	1.50	0.15	nm
Fundamental photon energy, E_{photon}	0.828	8.271	KeV
FEL saturated power, P_{sat}	11.0	9.6	Gwatt
Bunch duration, t_{bunch}	233	233	fsec
Position from undulator center, z	65.00	65.00	m
Fundamental transverse FWHM	232.7	86.7	micron
Peak photon density, A_{peak}	315	199	photons/nm^2

The transverse FWHM is the distance along x or y were the projected beam profile takes on half of its peak value. It is given by $FWHM = \sqrt{2 \cdot \ln(2)} \cdot w(z)$.

Dose to low Z solids at absorber exit.

Dose calculations at the position of the absorber exit for the low Z solids are presented in figure 3. The horizontal axis is the energy of the FEL fundamental photon beam.

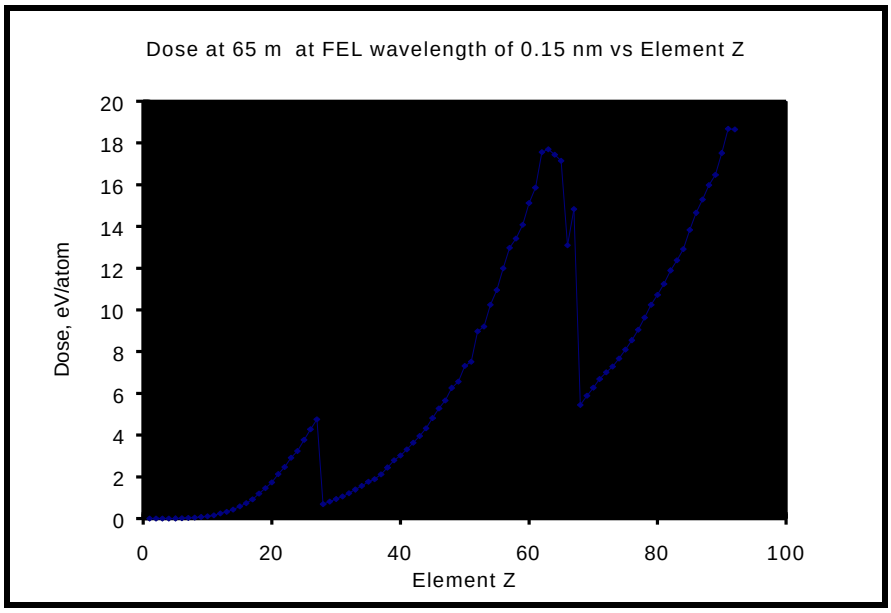


• Figure 3: Calculated dose to low Z solids at absorber exit.

The vertical axis is the dose in units of eV / atom. As expected, Li surfers the lowest dose ranging from slightly over 0.1 eV/atom at 0.828 KeV to under 0.001 eV/atom at 8.271 KeV. In general the four lowest Z solids, Li, Be, B, and C form a group that has the lowest doses at all energies ranging from 0.1 to 2.0 eV/atom at the lowest photon energies to <0.02 eV/atom at the highest energies. The other low Z solids, Na, Mn, Al, and Si, have doses more than 10 x higher than the first group because these elements have an absorption

edge between 1 and 2 KeV. Near this edge the doses approach 10 eV/atom. Even at the highest photon energies the dose to these higher Z solids is between 0.1 and 1.0 eV/atom.

The situation will be much worse for the common higher Z solids used in x-ray optics such as Mo and Ta where doses will exceed 100 eV/atom at the lower photon energies. Even at the highest photon energy 8.27 KeV, the doses will exceed 1.0 eV/atom for all elements having atomic numbers > 15 as shown in figure 4 which is a plot of the dose at the absorber exit for each element at the maximum FEL energy.



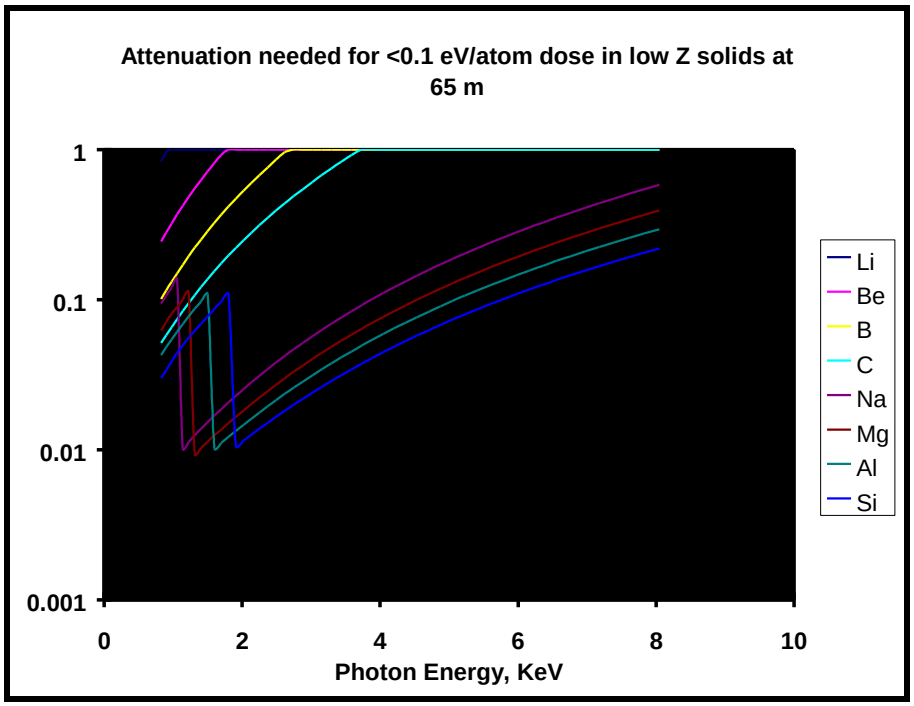
• Figure 4: Dose at absorber exit at 8 KeV

To interpret these dose plots it is necessary to know the damage threshold. Certainly ≥ 1 eV/atom, enough to ionize every atom, will disrupt sold structures. Doses of <0.01 eV/atom are probably safe. Experiments done at LLNL by Art Toor's group, using short optical pulses to quickly deposit energy into multilayer x-ray optical elements, showed that these structures were damaged at dose levels ≤ 0.1 eV/atom. Apparently the hydrodynamic shock resulting from the instantaneous deposition of energy into a small volume was enough to cause material to blow off of the surface. These experiments suggest that the damage threshold for solids is $\leq$ 0.1 eV/atom.

Until further experiments and/or calculations are done, in what follows I will take the damage threshold for solids to be between 0.01 and 0.1 eV/atom.

Attenuation needed to prevent damage to low Z solids at absorber exit.

Figure 5 shows the attenuation factors needed to bring the dose levels to each of the low Z solids at the absorber exit to 0.1 eV/atom vs. photon energy. The curves were obtained for each low Z sold by dividing 0.1 eV/atom by the dose calculated for that sold in figure 1. At photon energies where the solids have doses < 0.1 eV/atom the attenuation factor is given as 1.0.



• Figure 5 Attenuation needed to protect low z solids at absorber exit.

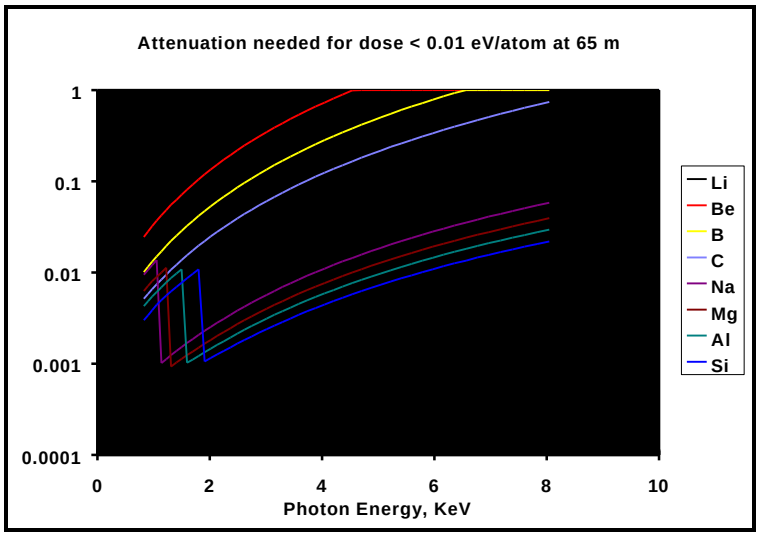
To stay below 0.1 eV/atom the lowest Z solids, Li, B, Be, and C, only require attenuation below photon energies of 0.92, 1.8, 2.7, and 3.7 KeV respectively. This is important, for if these materials are really not damaged at doses of 0.1 eV/atom, they could be used as primary attenuators and windows, greatly simplifying the design of other optical and safety systems. In particular, the more refractory elements B and C (especially the compound B_4C whose dose is < 0.1 for photon energies >2.9 KeV) are likely to have higher damage thresholds than most materials. Thus it would be very useful to have hydrodynamic calculations of the response of the lowest Z solids to instantaneous depositions of energy having the magnitude and spatial profile expected to be induced by the FEL pulse.

On the other hand, the oxide, BeO (not shown) , which will be present on the surfaces of any block of Be, requires a minimum photon energy > 4.7 KeV to suffer doses <0.1 eV/atom. Below photon energies of 4.7 KeV, the thin oxide coating on any Be optical elements is likely to spall off of the surface, which may be a safety concern.

The other solids, Na, Mn, Al, and Si, obviously require some attenuation even at the highest photon energies to stay below the 0.1 eV/atom damage threshold.

The next figure, 6, shows the attenuation needed to stay below the more conservative 0.01 eV/atom damage threshold. The 3 lowest Z solids, Li, Be, and B, are seen to be "safe" above photon energies of 2.6, 4.5, and 6.5 KeV. C, on the other hand, always requires some attenuation by this criteria since the dose to C is always > 0.01 eV/atom at any FEL wavelength. At 8.0 KeV C requires that the beam be attenuated by a factor of 0.7 to stay below the 0.01 eV/atom threshold.

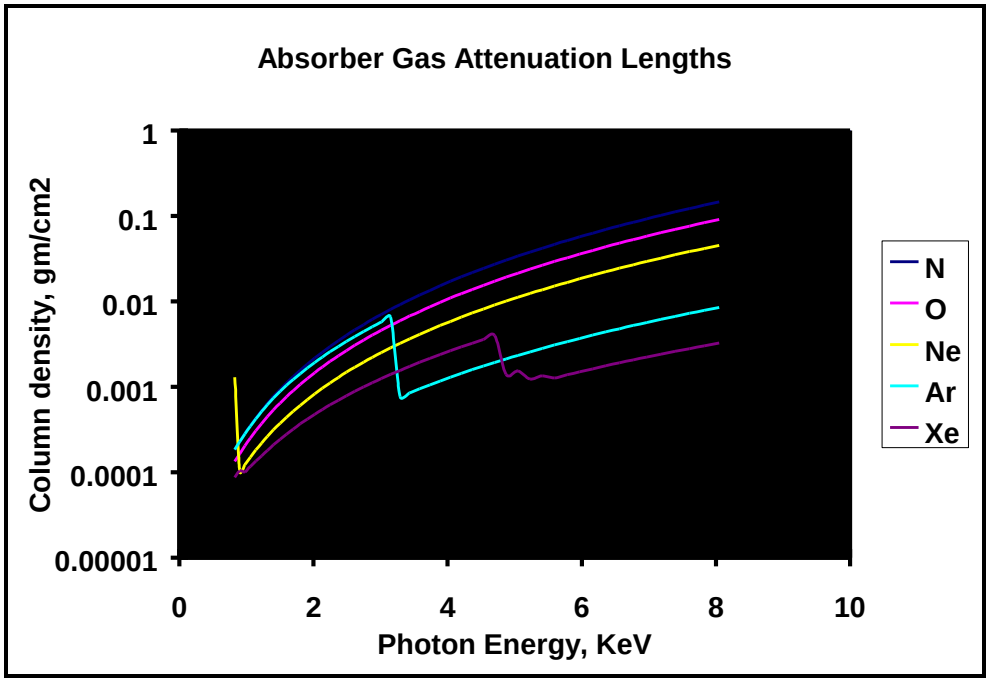
The other low Z solids, Na, Mn, Al, and Si, all require that the beam be attenuated to a few % or less of its raw intensity to stay below the 0.01 eV/atom threshold.



• Figure 6: Attenuation needed to protect low z solids at absorber exit using a conservative 0.01 eV/atom damage threshold.

Gas attenuator candidates

As candidate gases for the absorption cell, I have considered N, O, Ne, Ar, and Xe. Figure 7 shows the absorption length of these gases in units of column density, gm/cm^2.



• Figure 7: Attenuation lengths of candidate absorber gasses.

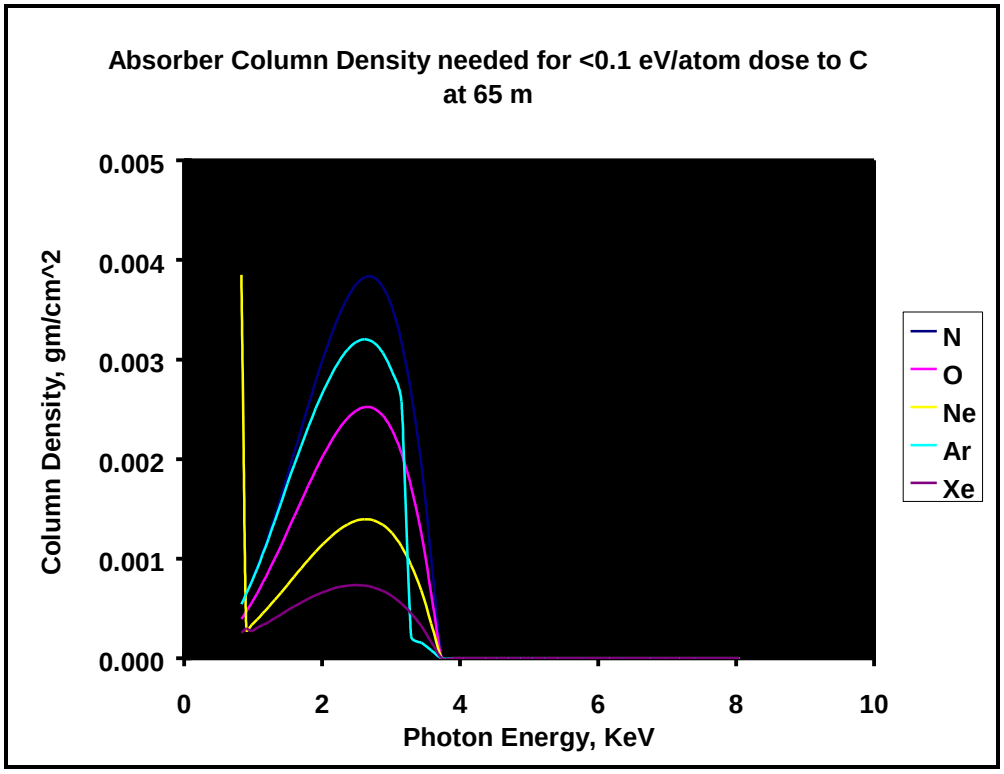
The highest attenuation lengths in these units are for the gases N and O which are the top two curves in this plot. The curve for Ne, in general has the third highest attenuation but for a sharp absorption feature below 1 KeV. The attenuation length for Ar has an

absorption feature around 3 KeV, and Xe shows an absorption feature around 4.5 KeV, above which it has the shortest attenuation length of the gases under consideration.

Safe gas attenuator densities for C optics

As seen above, the amount of attenuation needed to prevent damage to a given low Z solid is a function of FEL photon energy. Since the attenuation lengths of the candidate gases also vary with photon energy, a given low Z sold will require different gas densities at each photon energy to keep the dose less than the damage threshold.

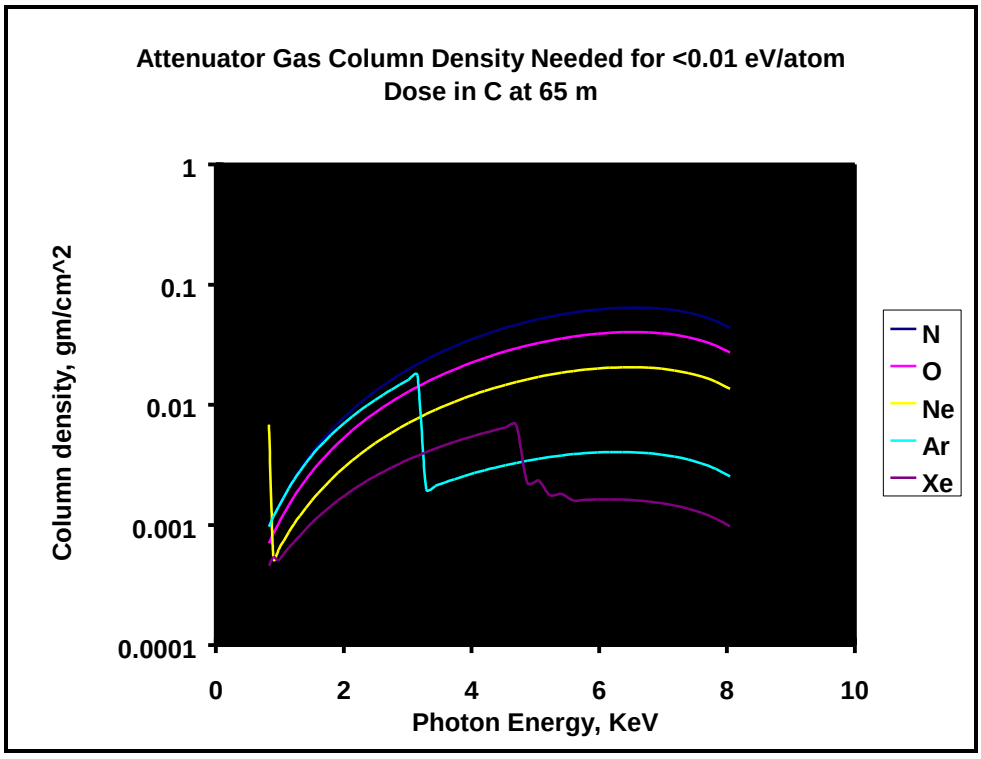
Consider the material C, which for various reasons may be the most practical low Z solid to use in the LCLS. For each candidate gas I have calculated the density necessary to prevent damage to C as a function of FEL photon energy. Figure 8 shows the result for the 0.1 eV/atom damage threshold.



• Figure 8: Absorber gas column densities needed to protect C at the 0.1 eV/atom damage threshold.

The curves in figure 8 are the column densities of each gas that will provide the "needed" attenuation specified in figure 5 for C at each photon energy. As the photon energy is increased, the required density becomes larger because the attenuator gas becomes more transparent. This trend is offset by the fact that at higher photon energies the dose to C goes down requiring less attenuator gas. Above 3.7 KeV, where the dose to C falls below 0.1 eV/atom, the required gas densities are zero since no attenuation is needed by the 0.1 eV/atom criteria. The most striking feature of the density curves is that the peak column densities are at photon energies around 2.6 KeV for all gases except Ne which has an absorption feature just above the minimum photon energy. The peak densities needed at 2.6 KeV in units of gm/cm^2 are 0.0038 for N, 0.0032 for Ar, 0.0025 for O, 0.0014 for Ne, and 0.00074 for Xe. Note that Ar, because of its absorption edge, requires higher density than O at 2.6 KeV. And Ne, because of its absorption feature requires a peak density of 0.0038 gm/cm^2 at the lowest FEL wavelength.

Figure 9 is a similar plot, of the column density needed to bring the dose to C to below the 0.01 eV/atom threshold at the absorber exit, but on a log-linear scale. Since the dose to C is always > 0.01 eV/atom at this location, finite column densities are needed at every FEL energy in order to lower the dose to 0.01 eV/atom.



• Figure 9: Absorber gas column densities needed to protect C at the 0.01 eV/atom damage threshold.

Ar and Xe supply sufficient attenuation above 5 KeV photon energy at column densities between 0.001 and 0.004 gm/cm^2 . The other gases, N, O, and Ne, require densities 10 X greater, in the range between 0.01 and 0.07 gm/cm^2 . Because of its absorption edge, Ar loses its high Z advantage at photon energies < 3.0 KeV and requires densities up to 0.02 gm/cm^2 to provide sufficient absorption below 3 KeV. Similarly, the required density for Xe is highest just below its absorption edge around 4.5 KeV reaching 0.007 gm/cm^2 .

These column densities are minimal in the sense that other solids with higher Z than C will require higher absorption to control the dose. If it is necessary to use the gas absorption cell to provide all of the absorption necessary to control the dose in other solids then gas densities 3 to 5 times higher will be required.

Certainly the gas absorber will be simpler to fabricate and operate if it is designed to operate only over a limited range of pressures which are as low as possible. A hybrid absorbing system using a limited gas cell to protect a bank of user selectable C absorbers might prove to be the most cost-effective solution.

Column densities that are safe for C at all FEL wavelengths

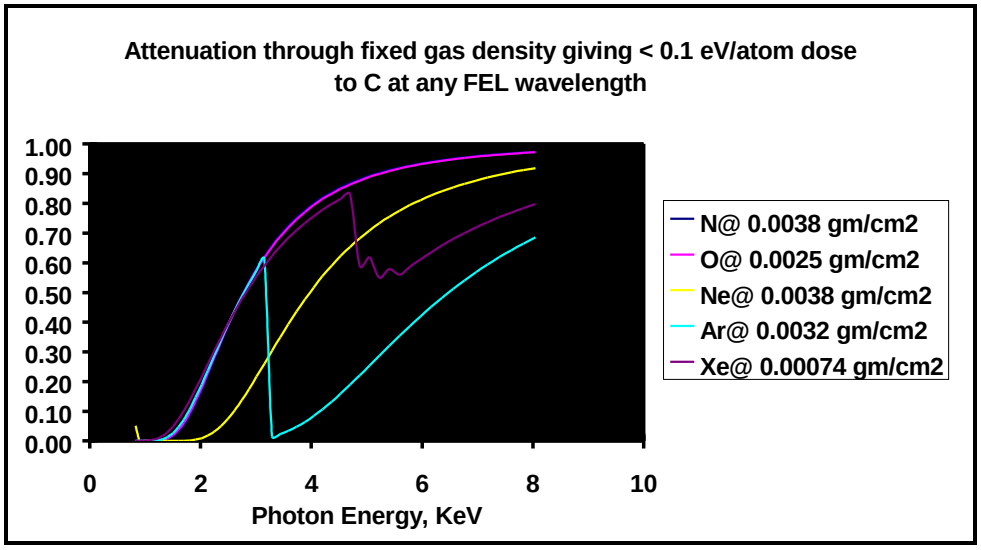
One could imagine that a more cautious user might want to run with a single fixed gas density in the absorber sufficient to protect his optics against damage no matter what FEL wavelength is delivered. This may also be necessary to assure safe operation in certain situations such as during studies of accelerator or undulator settings. For each gas, the single column density necessary to guarantee that the dose to C will always be < the given damage threshold at any FEL wavelength is the maximum density of the corresponding curves in figures 8 and 9. These are tabulated for the two damage criteria under consideration for each gas in the following table:

- Table 2: Maxim absorber column densities needed to protect C at absorber exit.

	0.1 eV/atom			0.01 eV/atom		
Absorber	**electron T, GeV**	**photon E, KeV**	**Safe x, gm/cm^2**	**electron T, GeV**	**photon E, KeV**	**Safe x, gm/cm^2**
N	8.04	2.6	0.0038	12.81	6.6	0.0644
O	8.04	2.6	0.0025	12.81	6.6	0.0404
Ne	4.54	0.83	0.0038	12.81	6.6	0.0205
Ar	8.04	2.6	0.0032	8.79	3.1	0.0176
Xe	7.89	2.5	0.00074	10.82	4.7	0.0068

Also shown in the table is the photon energy, and corresponding electron kinetic energy, where the maximum density is required to bring the dose to C to the threshold level. Running at other photon energies, but with these same fixed densities listed in the table, will be safe, but not optimal, since at other photon energies the fixed densities in the table will give greater attenuation than what is needed to reduce the dose to the damage threshold.

It is interesting to look at the attenuation through the "safe" fixed gas densities given in the table as a function of FEL photon energy. Figure 10 shows the attenuation as a function of photon energy for the fixed densities listed under the 0.1 eV/atom safe column in the table.

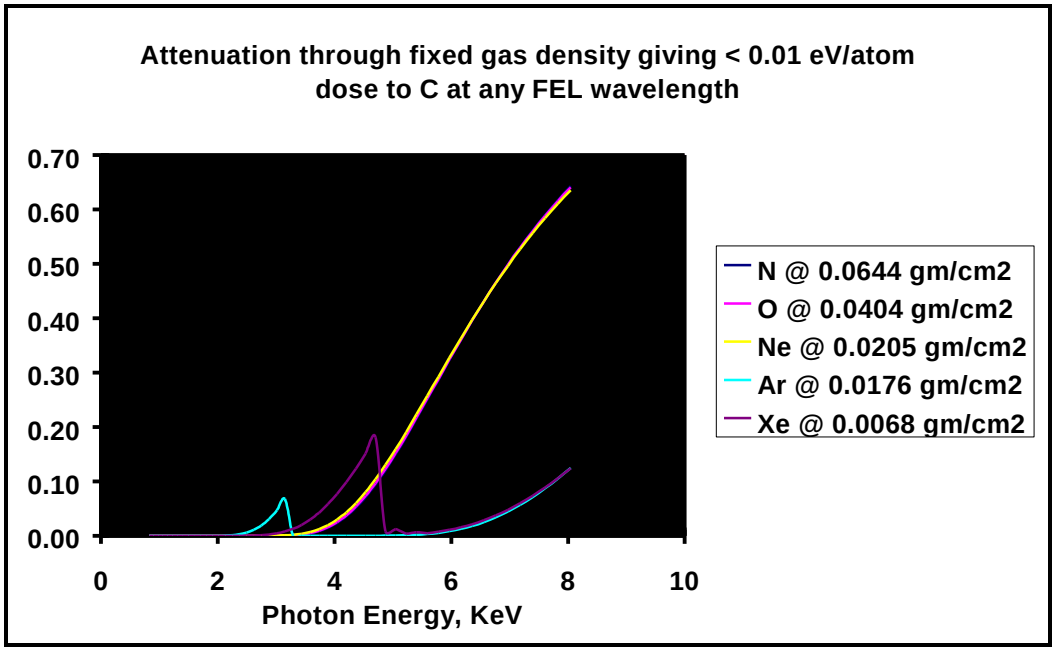


- Figure 10: Attenuation through the fixed gas densities in the first columns of Table 2.

Except for Ne, the attenuation curves for the gases cross at 2.6 KeV because at this photon energy the highest density of gas is needed, and that density gives the fixed amount of attenuation needed (~45%) to drive the dose to C down to 0.1 eV/atom. As

mentioned, at the other photon energies the attenuation is more than what is required to drive the dose down to 0.1 eV/atom. Because of absorbtion edges, the high Z gases Ar and Xe are more transparent at the 2.6 KeV photon energy where the most material is required, resulting in a higher "safe" fixed density. This higher fixed density is seen to over compensate at photon energies above the absorbtion edges. In particular at 8 KeV photon energy, where no attenuation is needed to get below 0.1 eV/atom, the attenuation of the safe densities of Ar and Xe are 60 to 70% while the low Z gases have attenuation above 90%. The low Z gases, N and O, do a much better job of matching needed attenuation with beam energy at fixed densities.

The effect is even more striking for fixed gas densities that keep the dose to C to <0.01 eV/atom as shown in figure 11. As indicated in Table 2, the maximum densities of N, O, and Ne, are needed at photon energies around 6.6 KeV. And absorber filled with this 6.6 KeV maximum density of N, O, or Ne would not only be safe at 6.6 KeV but would provide almost exactly the attenuation needed at higher photon energies. In contrast, an absorber filled with a fixed "safe" density of Ar or Xe would have to be filled with a high enough density to provide sufficient attenuation below their absorption edges resulting in pronounced absorption at higher energies and amounting to 10% transmission at 8 KeV.



• Figure 11: Attenuation through the fixed gas densities in the second columns of Table 2.

It would seem then, that for protecting C, at all photon energies, lower Z absorber gases are more favorable. This is not surprising because one would expect that the best absorber material for protecting a given sold would have the same absorption characteristics as the solid i.e. would have the same Z. If the sold is C, then absorbers with Z < 10 are optimal.

Dose to low Z solids at other locations

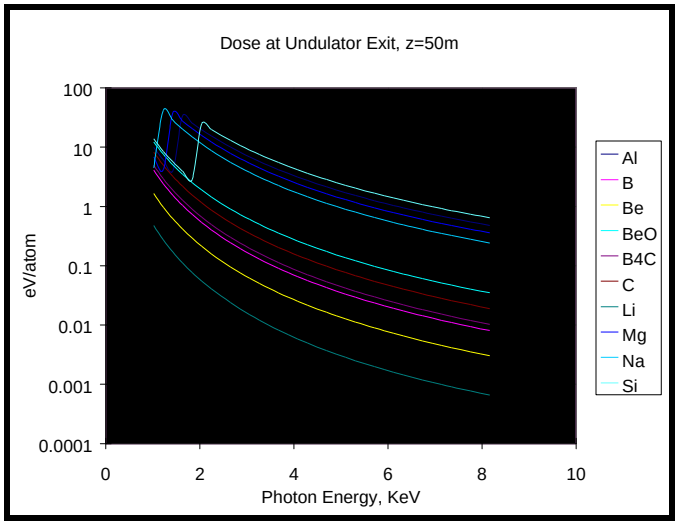
For reference, I present the doses to low Z solids at other positions of interest to users and developers of beam elements. The positions are: the exit of the undulator, the location of the proposed slit, the center of the gas absorber cell, the locations of the mirror and crystal tanks, and the general experimental area. These positions are summarized in the table which gives the distance of each position from the undulator center, and the FWHM and central photon densities at the minimum and maximum FEL energies.

- Table 3: FEL parameters along beam line.

FEL Photon Energy:		0.828 KeV		8.27 KeV	
	Z m	FWHM micron	A_{peak} /nm^2	FWHM micron	A_{peak} /nm^2
Undulator Exit	50.0	85	2351	72	290
Slit	59.9	179	532	81	225
Absorber Center	63.7	219	356	85	205
Mirror Tank	82.0	415	99	105	134
Crystal	84.4	441	88	108	128
Experimental Area	100	611	46	126	93

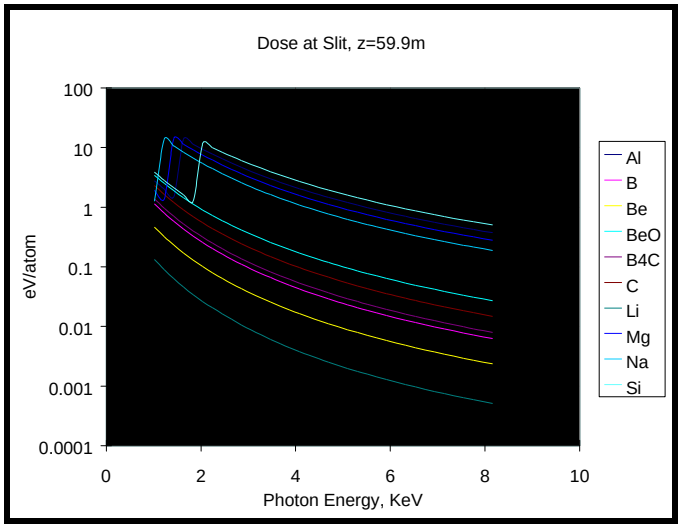
Figures 12 through 17 give the dose calculations for the low Z solids, as well as the compounds BeO and B_4C, at each location.

Because of the small divergence of the 8 KeV FEL beam, the doses at the highest energies do not change significantly with distance along the beam line. Be, B, B4C,C,and BeO surfer doses of the order of 0.01 eV/atom all along the beam line, and primary optical elements made of these materials, operating at high photon energies, can be used without fear of damage. The higher Z solids, Na, Mg, Al and Si suffer doses a factor of 10 higher, of the order of several 0.1 eV/atom. Optics made of these materials will likely be damaged by the primary beam anywhere along the beam line.



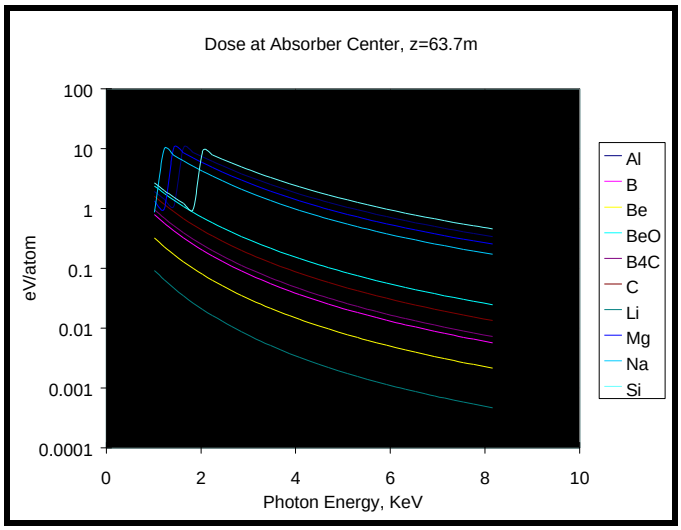
- Figure 12: Dose at undulator exit.

At the lower FEL energies, the larger beam divergence causes significant reduction in dose with distance along the beam line. At the closest position, the undulator exit, all materials, except perhaps Li, surfer doses sufficient to cause damage at photon energies at or below 5 or 6 KeV. Any type of optic or diagnostic placed in this position would also have to contend with the election beam.

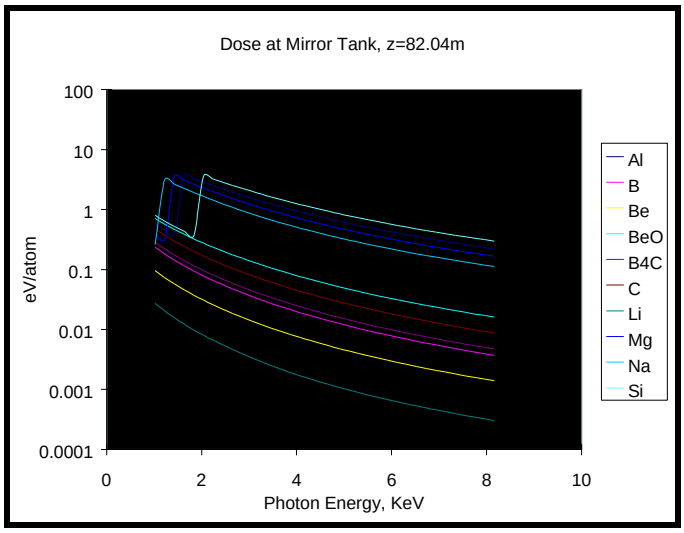


- Figure 13: Dose at slit.

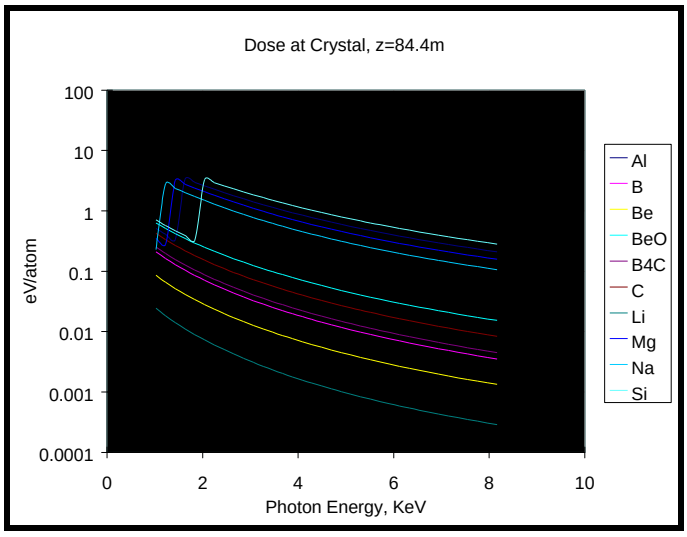
At the position of the slit, the dose to Be is below 0.1 eV/atom for photon energies above 2 KeV but the dose to its oxide is 10 times higher. Here it is important to know the exact threshold for damage (ablation) to Be and its oxide in situations where the slit or its fixturing surfer a direct hit from the primary beam.



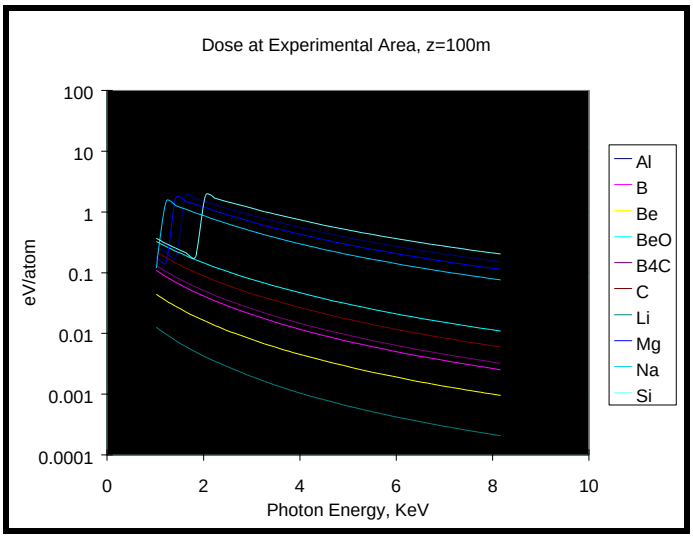
- Figure 14: Dose at absorber center.



- Figure 15: Dose at mirror tank position.



- Figure 16: Dose at crystal position.



• Figure 17: Dose at the experimental area.

These plots show that at lower FEL energies the doses are below 0.1 eV/atom for Be, B, B_4C, and C in the experimental areas.

Conclusions

These dose calculations show that the low Z solids Li, Be, B, and C are marginally at or below damage thresholds of 0.01 to 0.1 eV/atom at the positions along the beam line likely to contain optics.

To keep the dose to solid C below a conservative 0.01 eV/atom at the absorber exit requires absorber cell gas densities ranging from $\leq$ 0.007 gm/cm^2 for Xe to $\leq$ 0.07 gm/cm^2 for N. This density must be adjusted at each FEL energy to optimize throughput. The adjustment is especially important for the high Z gases Ar and Xe were absorption edges at the lower FEL energies require increased gas density.

It is possible to specify a fixed density of gases that renders the beam safe for C at all FEL energies. For this purpose, the lower Z gases are a better choice because low Z gases better match the absorption needed vs. wavelength resulting in a much more optimum throughput at the higher energies compared to fixed densities of Ar or Xe.

Finally, it is important to quantify the damage thresholds for the low Z solids. Great simplifications in the design of the absorber cell are possible if we can prove that the threshold for ablation in materials like Be, B, B4C, and C are $\geq$ 0.1 eV/atom.

Acknowledgement

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