LCLS-II Technical Note

Time-dependent simulation of the gas attenuator for the LCLS-II Xray FEL's under high beam power operations

LCLS-II TN-15-24

8/7/15

Y. Feng, J. Krzywinski, D. W. Schafer, E. Ortiz, M. Rowen, and T. O. Raubenheimer



ABSTRACT

Time-dependent simulation was carried out to study the dynamic response of a gas-based attenuator system designed for the LCLS-II high repetition rate X-ray Free-electron Laser's, and to further elucidate the impact of the fluctuating energies of proceeding pulses on the actual attenuation factor achieved for the trailing pulses. The filamentation effect in the gas density revealed from an earlier steady-state calculation under a constant Continuous-Wave input power was reproduced with additional ramping behavior and oscillations arising from the onset and the pulsed structure of the beam. More importantly, the actual achieved attenuation for a given pulse was found to vary randomly in response to the fluctuations in the input power.

Keywords: X-ray, FEL, simulation, gas, attenuator, filamentation

1. INTRODUCTION

X-ray attenuators are essential beamline components for providing safe and flexible operations. Various experimental conditions arise when the beam intensity must be reduced in a controlled manner before delivery to downstream user. For example, during detector alignment the full X-ray beam should not be applied unless the scattered intensity onto the detector is confirmed to be within the safe limit; using an attenuated beam and gradually increasing the beam intensity is a surefire experimental practice, which is especially important at Free-Electron Laser (FEL) facilities such as the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory because the extremely high peak intensity of the FEL beam can potential cause irreparable damages to equipment such as detectors if proper procedures are not strictly followed.

Building a high repetition rate X-ray FEL attenuator imposes additional specific requirements that it must not only withstand the extremely high peak intensity, but also dissipate the absorbed energy sufficiently quickly before the arrival of subsequent pulses. The former requirement is used to downselect techniques that can be applied. For example to attenuate a soft X-rays FEL beam a gas medium must be used. A typical gas attenuator consists of a long windowless tube filled with a gas of choice, such as N₂ or Argon, with the pressure adjusted for changing the attenuation. The gas tube is then connected on both ends to long differential pumping sections for maintaining ultrahigh vacuum conditions elsewhere. The fast energy dissipation requirement has often been overlooked and assumed to be satisfied as in the case of the gas attenuator built for the LCLS X-ray FEL with a maximum repetition rate of 120 Hz. There the inter-pulse separation of 8.3 ms is thought to be sufficiently long such that the gas volume returns to the original state before the next pulse, including mostly importantly the effective density "seen" by the X-rays. As such, there is a direct relation between the gas pressure and the prescribed attenuation, which can be calculated solely based on the total mass attenuation coefficient, density, and effective length of X-ray-gas interaction region.

For future high repetition rate X-ray FEL's the minimum inter-pulse separation is reduced significantly by 4 orders of magnitude to 1.0 us for LCLS-II at 1 MHz or 0.22 us for European XFEL at 4.5 MHz within a macro-pulse. These time scales are presumed to be too short for the entire gas volume to relax completely back to its starting conditions. Consequently, the trailing pulse will likely encounter a higher temperature and thus a lower density condition because of the heating by the absorbed power. The actual attenuation will be lower and will depend on the prior history of energy deposition and thermal relaxation in the system and cannot be predetermined by a simple calculation using the equilibrium gas pressure alone, as opposed to how it is done when using the attenuator under low repetition rate operation. This gas "filamentation" or density depression phenomenon by preceding pulses has been reported by Cheng, et. al.1 using an ultrashort optical laser. They observed that a lower-density filament with both radial and axial extent was created in a 1-atm N₂ gas cell, which was irradiated by an 800 nm Ti:Sapphire laser beam of 100 μ m in diameter, producing an average energy of 0.72 mJ/pulse at a repetition rate of 20 Hz. The density depression in the filament was as high as 20% and the recovery time was approximately 1 ms, as measured by using an interferometric technique after a single pulse. The optical laser parameters were very similar to the LCLS FEL beam, and a similar density depression effect would have likely existed in the LCLS gas attenuator, and was perhaps completely unbeknownst to anyone due to the lack of any substantial operational consequences or experimental inquiries.



Figure 1. Schematic of the geometry for the time-dependent simulation of the gas-based attenuator, which is 20 mm $(2R_p)$ in diameter and 5 m (L_p) in length, and is filled with Argon gas regulated to pressure *P* and has its outer walls cooled to 300 K (T_0) . The FEL beam has a diameter of 2 mm $(2R_b)$ and a pulse repetition rate *F*.

The LCLS-II soft (200 to 1300 eV) and hard (1 to 5 keV) X-ray FEL's are being designed to operate up to 1 MHz in a Continuous-Wave (CW) mode and to generate pulses with comparable energy of a few mJ. The maximum time-averaged FEL power, however, will be purposely limited to 200 Watts by a combination of reducing the repetition rate and/or using a lower electron bunch charge for producing lower per-pulse energy. The baseline design for the LCLS-II gas attenuator2 will be of the same concept as that of LCLS, consisting of a 5 m long tube filled with Argon gas with a maximum operating pressure of < 10 Torr shown schematically in Figure 1. The "filamentation" effect is expected to be present and must be properly studied, understood, and mitigated. In this report, we present a time-dependent finite-difference thermodynamic analysis to augment the findings from an earlier steady-state calculation under a constant CW input power3 and to elucidate the impact of the fluctuating energies of proceeding pulses on the actual attenuation factor achieved for the trailing pulses. In addition to reproducing the same "filamentation" effect, the dynamic responses of the gas attenuator were obtained, including the temperature ramping and oscillations arising from the onset and the pulsed structure of the beam. More importantly, the actual achieved attenuation for a given pulse was found to vary randomly in response to the fluctuations in the input power.

2. Thermodynamic Simulation

The interactions between a femtosecond X-ray FEL pulse and the molecules in a dilute gas are very complex and are the subject of many pioneering experimental studies 4.5. However, for our thermodynamic simulation we assume that after the initial photoionization of a small percentage of the molecules, many fast electronic processes including Auger decay, inelastic collisions, impact ionization, attachment, recombination, etc. would help thermalize the energy of the fast primary electrons into the thermal energy of all free electrons (primary and secondary), ions and other excited molecular species. This thermalization process should be complete on a time scale of a few to tens of picoseconds. According to Cheng, et al.¹, what follows on a time scale of a few to tens of nanoseconds is the repartitioning of the energy in the electronic/ionic/molecular excitations degrees of freedom into an essentially fully recombined gas in its ground electronic state. The result of the repartitioning will create a temperature gradient, which in turn creates a pressure gradient since the local (by now fully recombined) gas density remains more or less unchanged on time scales shorter than a few nanoseconds. Given the gas attenuator's large length-overradius ratio depicted in Figure 1, both the temperature and pressure gradients are mostly in the radial direction. This pressure gradient will drive a hydrodynamic motion of the gas in the form of density waves on a time scale of tens of nanoseconds to a few microseconds to eventually establish a constant pressure (after the hydrodynamic motion of the molecules arising from the pressure gradient all but ceased, i.e., macroscopic fluid velocity $v \sim 0$). At the end of pressure equilibration, a quasi-equilibrium is reached where the temperature gradient remains largely unchanged, but a density profile or depression develops over the same length scale set by the temperature gradient. Further evolution of the gas in temperature and density will be thermal diffusion dominated on time scales ranging from a few microseconds to a few milliseconds or even longer and is the focus of the present thermodynamic analysis.



Figure 2. (Top left) Equilibrium temperature profiles in the radial direction at various z positions. (Top right) Equilibrium temperature profile in the axial direction at the center of the attenuator at r = 0 mm. (Bottom left) Equilibrium normalized density profiles in the radial direction at various z positions. (Bottom right) Equilibrium normalized density profile in the axial direction at the center of the attenuator at r = 0 mm. The simulation was done for an Argon gas attenuator attenuating a 200 eV soft X-ray FEL beam of 200 W average power by a factor of 10^5 .

2.1 Steady-state solution for constant CW input power

The first thermodynamic simulation³ was performed assuming the gas has reached a steady-state equilibrium distribution under a constant CW input power, while the second simulation reported in this paper aimed to elucidate the time-dependent aspect of density and temperature gradients in between the pulses, from which the actual attenuation for any given pulse can be evaluated. The first case represents the asymptotic solution $(t \rightarrow \infty)$ of the second one when the repetition rate of the FEL approaches infinity while the per-pulse energy becomes infinitesimally small but keeping the total input power constant. For simulation purposes, the gas attenuator was idealized as shown in Figure 1 to be a 5 m long and 20 mm in diameter tube filled with Argon gas regulated to an equilibrium pressure P and impinged on by a 200 eV soft X-ray FEL beam of 2 mm in diameter. The FEL pulses are 50 fs long and 2 mJ in energy, and the repetition rate is 100 kHz, producing an average beam power of 200 W. The walls of the gas tube are cooled and kept at a constant temperature of $T_0 = 300$ K. Based on discussions above, we further assume that the thermalization (\leq a few ps), repartitioning (\leq a few ns), and pressure equilibration ((\leq a few μ s)) processes are all spatially confined to the region of the initial energy deposition which can be considered as instantaneous and is given simply by the transverse profile of the FEL beam. In the pressure range the gas attenuator will be operating in and on time scales longer than pressure equilibration, the Argon gas can be treated as an ideal one, and the local temperature $T(\mathbf{r}, t)$ and the density $n(\mathbf{r}, t)$ are well-defined variables that always conform to the relation that $n(\mathbf{r}, t)T(\mathbf{r}, t) = n_0(P)T_0 = P/k_B$, where T_0 and $n_0(P)$ are the background temperature and density at the pressure *P*. When the pulse structure of the FEL is replaced by a CW input of equivalent average power and after the gas has reached a steady-state condition that the local temperature and density are no longer changing in time, i.e., $T(\mathbf{r}, t) = T(\mathbf{r})$, and $n(\mathbf{r}, t) = n(\mathbf{r})$, the relation $n(\mathbf{r})T(\mathbf{r}) = n_0(P)T_0 = P/k_B$ still holds. The Fourier's law for heat transfer $\mathbf{J} = \kappa \nabla T$ is then utilized in solving the equilibrium temperature distribution $T(\mathbf{r})$ and by assuming that the energy deposition is limited to within the footprint of the beam and thermal transport is primarily in the radial direction by virtue of the very large aspect ratio of the tube geometry.

The findings of the CW input simulation can be found in a separate report³. Here we briefly discuss a specific case for a targeted attenuation factor of 10⁵, in which the "filamentation" or density depression effect reported by Cheng et. al.¹ was clearly reproduced. The equilibrium temperature profiles T(r, z) in the radial direction at various z positions are plotted in the top-left subpanel of Figure 2. The temperature at the entrance of the tube is elevated to as high as 1800 K at the center, and decreases gradually towards the sidewall, which is cooled to a constant temperature T_0 of 300 K. Temperatures at different z locations show similar radial dependence with the central maxima traced out by the curve in the top-right subpanel. Consequently, the normalized density profiles in the bottom-left subpanel show radial depression with central minima given by the curve in the bottom-right subpanel. The maximum depression at the center of the entrance amounts to approximately 30% of the density $n_0(P_0)$ required to provide the targeted 10⁵ attenuation factor with $P_0 = 1.43$ Torr being the equilibrium pressure if no filamentation effect is present. This deficit in density in the first half of the gas cell is then compensated by the surplus in the second half, and in fact the integrated area under the curve in the bottom-right subpanel exactly equals $n_0(P_0)L_0$ as expected. To provide the extra density the equilibrium pressure P has to be raised to 2.51 Torr from the low-power limit P_0 by a factor equalling the asymptotic value of 1.76 at $z = L_0$. The operating pressure P in relation to the low-power limit P_0 depends on many physical attributes of the attenuator and the beam, including the radius and length of the gas cell, the size and transverse profile of the beam and its average power. As such, the achieved attenuation cannot be simply calculated by using the equilibrium pressure alone as it would in the low-power limit. In principle, a very complex lookup table between the actual attenuation and other relevant parameters could be established experimentally first and then referenced to by subsequent routine operation. In practice, however, there are various fluctuations in the beam itself. including most importantly the pulse energy and thus the moving average power. Such fluctuations make the actual attenuation essentially unpredictable. The extent and the time scale on which this random behavior would impact the performance of the attenuator is the focus of the time-dependent simulation to be discussed next.

2.2 Time-dependent simulation of equal pulse energies

When the pulse nature of the FEL beam must be taken into account, the simulation for a CW input in Sect. 2.1 is no longer sufficient in understanding the time-dependent behavior of the system. These include the system relaxation time for the entire attenuator to ramp up to the steady-state distributions shown in Figure 2 and the inter-pulse relaxation process as to how the local temperature and density change after each pulse. The inter-pulse relaxation is important to understand the effect of the density depression created by the proceeding pulses would have on subsequent pulses in terms of the actual achieved attenuation and associated uncertainties. This is especially important when the pulse energy fluctuates randomly as in the case of most X-ray FEL lasers. It will be shown later that for a simple system depicted in Figure 1, which filled with a few Torr of Argon gas at room temperature, its thermal relaxation time is of order a few milliseconds. As such, if the repetition rate of the FEL beam is greater than 1 kHz, the gas medium in the attenuator does not have sufficient time to relax completely back to its starting condition after each pulse. However, it is still possible for the system to eventually establish a dynamic "steady-state" after many milliseconds if each pulse is identical, and the time-dependent behavior of the system simply repeats itself after each pulse. For example, the temperature at any given location is expected to rise and fall about the equilibrium temperature derived from the CW simulation, and the deviation depends on the repetition rate and the pulse energy. If, however, the pulse sequence has additional time scales in it, such as the macro pulse structure of the European XFEL beams, then the transient behavior of the system should also reflect these time scales as well.



Figure 3. (Top) Time evolution of the temperature at the center of the entrance of the attenuator (r = 0, z = 0 mm). The simulation was for an Argon gas attenuator for attenuating a 200 eV soft X-ray FEL beam of 2 mJ/pulse running at 100 kHz, producing an average power of 200 W. The targeted attenuation was set for 10^5 , for which the pressure was adjusted to 2.51 Torr as obtained by the CW calculation, 1.76 times higher than the low-power limit of 1.43 Torr. The red dashed indicates the equilibrium temperature for the CW case of equal average power at 200 W. The inset shows the 20 pulses between 1.8 and 2.0 ms. (Bottom left and right) Time evolutions of the temperatures at z = 2000 and 5000 mm, respectively, showing different relaxation constants. The different time scales at different z locations are due to the temperature dependence of the thermal conductivity κ .

To perform the time-dependent simulation, the homogeneous heat equation¹ in the differential form $\rho C_p \partial T/\partial t - \kappa \nabla^2 T = 0$ was solved similarly as in the steady-state case³ for an Argon filled gas attenuation for attenuating a 200 eV soft X-ray FEL beam of 2 mJ/pulse running at 100 kHz and time-average power Q of 200 W. Two similar assumptions were made: a) the transverse beam profile is of a flattop shape with an integrated pulse energy equivalent to that of the actual Gaussian-like beam; b) heat transfer is absent in the azimuthal direction due to symmetry, but is predominantly in the radial direction and thus negligible in the axial direction because of the large aspect ratio of the gas tube.

Assumption b) allowed the numerical simulation to be carried out by dividing the gas volume into thin disks of thickness Δz as depicted in Figure 1 and solving a one-dimensional partial differential equation for T(r, z) in variable r in a cylindrical coordinates starting from the beginning of the gas cell. The temperature profile was solved sequentially for each (*i*-th) disk starting from the first one at $z_i = 0$, with boundary conditions $T(r = R_p, z) = T_0$ at the walls and the initial $T(r, z_i, t = t_m^+)$ conditions which were derived after the *m*-th pulse. The rise in temperature $\Delta T(r, z_i, t = t_m^+)$ immediately after each pulse within the energy deposition volume was considered as instantaneous, certainly much faster than the time scale of pressure equilibration. The energy deposition was calculated based on the density profiles $n(r, z_i, t = t_m^-)$ of all proceeding disks ($z < z_i$) at the instant before the *m*-th pulse, which was obtained by using the local equilibrium condition $n(r, z_i, t = t_m^-)T(r, z_i, t = t_m^-) = P/k_B$ where P is the equilibrium pressure established throughout the entire gas tube. For the Argon gas used in the simulation, the isobaric molar heat capacity $C_p = 5R/2$ was used, where R = 8.31 J/mol·K is the gas constant. For non-monatomic molecules, C_p

¹ Unlike the steady state simulation, heat generation is absent other than the energy deposition immediately after each pulse, thus the source term is null if the heat equation is solved only in between pulses.

gradually become excited. For a concentric ring (with its outer radius $\langle R_b \rangle$ of height Δz located at $r_j \langle r \langle r_i + \Delta r \rangle$ and z_i , $\Delta T(r_i, z_i, t = t_m^+) = \Delta \varepsilon / (nC_p)$, where $\Delta \varepsilon$ is the pulse energy absorbed in the ring given by

$$\Delta \varepsilon = i \left(r_j, z_i \right) \left\{ 1 - \exp \left[-\frac{T_0 P}{T\left(r_j, z_i, t_m^- \right) P_0 L_0} \Delta z \right] \right\} \pi \left[\left(r_j + \Delta r \right)^2 - r_j^2 \right]$$
(1)

 $n = \pi[(r_j + \Delta r)^2 - r_j^2]\Delta z P/[RT(r_j, z_i, t = t_m]]$ is the number of moles of Argon in the ring, L_0 is the attenuation length of the gas at reference temperature T_0 and reference pressure P_{ref} , P(0) is the starting equilibrium pressure in the low power limit and $i(r, z_i)$ is the pulse intensity profile of the FEL beam at z_i . After substituting the (molar) density of ideal gas P/(RT) the differential heat equation for the *i*-th disk becomes:

$$\frac{5}{2} \frac{P}{T(r_j, z_i, t > t_m^+)} \frac{\partial T(r_j, z_i, t > t_m^+)}{\partial t} = \frac{1}{r_j} \frac{\partial}{\partial r} \left(\kappa r \frac{\partial T(r, z_i, t > t_m^+)}{\partial r} \right) \Big|_{r_i}$$
(2)

where the terms on right-hand-side (RHS) that represented heat transfer in azimuthal and axial directions have been neglected, and $\kappa = \kappa_0 \sqrt{T/\sqrt{T_0}}$ is the temperature dependent thermal conductivity of the (ideal) gas referenced to κ_0 at a reference temperature chosen for convenience as the constant temperature T_0 . Eqn. (2) is solved by stepping through small time steps, with the step size determined by the stability condition that it is smaller than the diffusion time set by the diffusivity of the gas and the mesh size Δr . Only after $T(r, z_i, t)$ was solved the pulse energy profile $i(r, z_{i+1})$ for the i+1-th disk could be calculated and used for solving the temperature profile $T(r, z_{i+1}, t)$. The density profile $n(r, z_i, t)$ was obtained by using the local equilibrium condition $n(r, z_i, t)T(r, z_i, t) = P/k_{\rm B}$ and used for calculating the actual achieved attenuation A(Q) for the trailing (m+1-th) pulse. This in practice was simply calculated from the pulse energy at $z = L_p$ by integrating the pulse energy profile $i(r, L_p)$, which has already been calculated with the fully evolved temperature profile at t_{m+1} . The density profile could also be normalized to that at constant temperature T_0 and equilibrium pressure P(0) in the low power limit for comparison.

As the average input power $Q \rightarrow 0$, the achieved attenuation A(0) is expected to be approach a value that can be simply calculated by using the equilibrium pressure in the low power limit. As the power increases, the actual achieved attenuation A(Q) will be reduced and the pressure must be increased to compensate the filamentation effect. Instead of finding the eventual pressure by iteration, here we simply used the equilibrium pressure obtained in the CW input steady-state simulation at 2.51 Torr rather than the low power limit of 1.43 Torr. The time evolution of the temperature in the gas tube is shown in Figure 3 for various z locations. The temperature at the entrance in the top subpanel shows an initial ramp and then plateaus while oscillating between a lower bound of ~1450 K and an upper bound of ~2370 K bookending the equilibrium value of ~1800 K (red dashed line) obtained for the CW input case shown in the top-left or top-right subpanel of Figure 2. This is expected as the equilibrium temperature of the CW input represents the asymptotic temperature when the repetition rate is increased while reducing the per-pulse energy but keeping a 200 W constant average power.

The time scale of the initial ramp-up process is of order 1 ms, substantially greater than the inter-pulse time of 10 µs, which is the total relaxation time after each pulse in the steady-state equilibrium. These two time scales should be related to the two length scales through the thermal diffusivity. Let us investigate the time evolutions shown in Figure 4, where in the left subpanel the temperature profiles in the radial direction are plotted in 1 us steps immediately after the passage of the first pulse, and the right panel after the *n*-th pulse after reaching steady-state equilibrium. Since there is no initial temperature gradient, the energy deposited within the (flattop) beam footprint stays near the origination location and gradually builds up the temperature gradient, which in turn helps promote energy transfer to locations closer to the wall. This build/transfer process is slower and its time scale t_1 is set by the thermal diffusivity $\alpha (= \kappa / \rho \cdot C_p =$ $2\kappa_0 T^{3/2}/(5\sqrt{T_0P}) = 0.126 \text{ m}^2/\text{s})$ of the Argon gas at 2.51 torr and an average temperature of ~1800 K and the typical length scale l (= 10 mm) of the relevant attenuator geometry via the scaling relation $t_1 \sim l^2/\alpha \sim 0.8$ ms. The estimate of t_1 is in excellent agreement with the time scale of the ramp-up shown in the top subpanel of Figure 3, which displays a slower rise and then a faster plateauing process, reflecting the temperature dependence in α . This also explains the much slower temperature ramp-ups at z = 2000 and 5000 mm in the bottom subpanels of Figure 3, where the average temperature is much lower than at the entrance of the attenuator at z = 0. For the steady-state equilibrium case the time scale is set by the interpulse time of 10 μ s. This is related, through α , to the length scale of ~ 1.1 mm. Indeed, it can be seen in the right panel of the Figure 4 that significant time variations of the temperature profile take place only close to the energy deposition region and 1 mm form the edge of the irradiation profile the time variations practically vanish. This apparent speed-up in the right subpanel of Figure 4 is attributed to the fact that energy transfer happens continually from r = 0 to the wall and everywhere in between, in contrast to what happens at the very beginning after the first pulse when the energies of many pulses have to move from r = 0 all the way across to the wall at r = 10 mm to build up the equilibrium profile given by the cyan dashed line in the left subpanel. In fact, it takes on the order of 100 to 200 pulses worth of energy to set up the necessary temperature gradient.



Figure 4. (Left) Time evolution of the temperature in the radial direction at the entrance of the attenuator (z = 0 mm) in 1 µs steps after the passage of the first pulse. The red line indicates the temperature distribution at t_1^+ , immediately after the energy deposition by the first pulse in the gas tube. (Right) Time evolution of the temperature in the radial direction at the entrance of the attenuator (z = 0 mm) in 1 µs steps after the passage of the 200-th pulse after reaching steady state equilibrium. The red line indicates the temperature distribution at t_{200}^+ , immediately after the energy deposition by the 200-th pulse. The simulation was for an Argon gas attenuator attenuating a 200 eV soft X-ray FEL beam of 2 mJ/pulse running at 100 kHz, producing an average power of 200 W. The targeted attenuation was set for 10⁵, for which the pressure was adjusted to 2.51 Torr as obtained by the CW input calculation, 1.76 times higher than the low-power limit of 1.43 Torr. Also note that the temperature profiles just before the 200-th (cyan-dashed line) and the 201-th (blue solid) pulse virtually overlap, signifying the reaching of steady state equilibrium.

To evaluate the actual achieved attenuation, it should be recognized from the top subpanel of Figure 3 that any given trailing pulse "sees" only the lower bound temperature thus higher density. It will encounter a higher attenuation factor of 2.5×10^5 than the one given by the CW input simulation at 1×10^5 in the steady state. As such, the dynamic value for the required pressure to achieve the targeted 10^5 attenuation should be somewhat lower than 2.51 Torr. Moreover, during the entire temperature ramp-up, the attenuation achieved for each pulse also undergoes a corresponding ramping process, starting at 5.8×10^8 for the first pulse, reflecting the fact that the entire gas cell started out cold, and the density was higher. If repeating the same simulation at half the repetition rate but twice the pulse energy, the system has 20 µs as opposed to 10 µs to relax from a higher upper temperature and thus reducing the required pressure further. This is made possible by virtue of the temperature dependence of the thermal conductivity of an ideal gas, which is proportional to \sqrt{T} . In fact if the repetition rate is sufficiently low so that the gas medium has sufficient

time to return to the starting conditions before the arrival of the next pulse, the required pressure should approach the low power limit even through the average input power is still constant at 200 W. However, this extrapolation could breakdown if the per-pulse energy (hypothesized at a low repetition rate but a constant power) becomes so high that our entire analysis may require certain refinement.

2.3 Time-dependent simulation of random pulse energies

The above simulation in Section 2.2 has been carried with equal per-pulse energy at 2 mJ/pulse. If the pulse energy varies randomly as for any Self Amplified Spontaneous Emission6⁻⁷ (SASE) X-ray FEL beam such as the LCLS or LCLS-II, the evolution of the temperature and density in between the pulses will fluctuate about the steady state equilibrium that the transient behavior no longer repeats itself. One of the significant consequences of this random behavior is that the achieved attenuation becomes less predictable even if with using a lookup table. A new simulation was carried out again for attenuating a 200 eV soft X-ray beam but with random input pulse energies, and used an initial temperature distribution obtained in the steady state CW input case in Section 2.1. The targeted attenuation was again set for 10^5 by setting the pressure to 2.51 Torr. To emulate the SASE stochastic behavior, the pulse energy was randomized from 0 to 4 mJ with an average of 2 mJ and a uniform distribution using a standard pseudorandom scalar generator function.



Figure 5. (Top) Time evolution of the temperature at the center of the entrance of the attenuator (r = 0, z = 0 mm) with randomized input pulse energies. The simulation was for an Argon gas attenuator for attenuating a 200 eV soft X-ray FEL beam of random pulse energies, which were uniformly distributed between 0 and 4 mJ with an average of 2 mJ, producing an average power of 200 W. The targeted attenuation was set for 10^5 , for which the pressure was adjusted to 2.51 Torr as obtained by the CW calculation, 1.76 times higher than the low-power limit of 1.43 Torr. (Bottom) The actual achieved attenuation for each pulse, which also varies randomly in response to the fluctuating pulse energy.

The temperature evolution at the attenuator center (r = 0, z = 0 mm) for the randomized input is shown in the top subpanel of Figure 5, where temperature still oscillates about a certain mean value, but with an increasing degree of randomness, in strong contrast to those nearly periodic "quick rise-and-slow decay" curves in the inset of top subpanel of Figure 3. Correspondingly, the density profile that the ultrafast X-ray FEL pulses would "see" upon arrival will fluctuate, leading to large variations in the actual achieved attenuation, shown in the bottom subpanel of Figure 5, by as much as 70% peak-to-valley (i.e., 5×10^5 at pulse #155 and 2×10^5 #185). There is, however, no direct correlation between the temperature and attenuation fluctuation on a pulse-by-pulse basis for a simple reason that the entire gas attenuator responds to the input pulse energy in a delayed and time-averaged manner set by the time constant t_1 not t_2 . The attenuation of any given pulse depends implicitly on each and every proceeding pulse and its energy and the exact arrival sequence, if the other parameters of the attenuator are kept constant. If the cooling conditions on the boundary wall changes, or the pressure deviates from the set point, the achieved attenuation would encounter additional fluctuations. In the end, the pulse energy after the attenuator must be measured independently, and the lookup table established experimentally may serve merely as a guide for how much attenuation the pulses would ultimately receive. The intensity fluctuations is of order 10 to 20% in a typical well-tuned SASE beam but 100% in the seeded operation, the variation in the attenuation will likely be somewhat less than 70% peak-to-valley, but will not likely be better than 20%. A similar simulation for a Gas Monitor Detector8 (GMD) downstream of the attenuator would give us some confidence that the depression effect is insignificant on the GMD performance, so we are be able to rely on it as the mitigation to the filamentation effect on the attenuator.

3. Conclusions

Both static and dynamic effects of filamentation or density depression in a gas attenuator serving a high repetition rate X-ray FEL beam were demonstrated numerically using a finite difference method. For the static filamentation simulation, a constant CW input was used. It was found that for a given gas cell geometry (thus its effective dimensionality) and a set of boundary conditions, the steady-state equilibrium temperature distribution depends, according to the Fourier's law for heat transfer $J = \kappa \nabla T$, only on the thermal conductivity of the gas medium, which itself may be temperature dependent, thus producing additional nonlinear behavior. Filamentation phenomenon occurs because of a gas medium possessing the ability to expand substantially at elevated temperatures unlike a solid or liquid matter. The equilibrium (static) temperature profiles such as those shown in Figure 2 require the use of a self-consistent approach to solving the heat transfer equation. One important assumption made was that an equilibrium pressure has been established globally, and that there was always local equilibrium between temperature and density regardless of the time scale. For a CW input this assumption works well, and for a pulsed FEL beam it remains valid if the time for pressure equilibration is much faster than the inter-pulse separation. The degree of the static filamentation exhibited complex relationship to many physical attributes of the system, including the gas species, pressure, input power, desired attenuation, and geometries of both the beam itself and the attenuator. As such, the simple and direct correspondence between the gas pressure and prescribed attenuation, often assumed for a sufficiently low repetition rate (thus necessarily low average power) FEL beam, breaks down. In principle, a lookup table can be established for guiding the attenuator operation if not considering the fluctuating pulse energy.

The evolution of the filamentation was elucidated by carrying out time-dependent finite difference simulations, assuming constant pulse energies and starting from a cold condition when the entire gas volume was at the temperature of the walls. Two time scales were found, one related to time to ramp up to the steady state equilibrium distributions, and one related to the relaxation process between pulses. The former depends only the thermal diffusivity $\alpha = \kappa / \rho \cdot C_p$ of the gas medium and the typical length scale of the cell geometry. It is worth noting that the specific heat C_p of the gas is completely absent in working out the steady-state solution, but changes the time scales of the dynamic effects. The smaller the specific heat is, the faster the ramp-up time. When the input pulse energy fluctuates as is the case for all SASE based Xray FEL sources, the shape and depth of the filamentation responds to the changing pulse energies not on a pulse-by-pulse basis but in a delayed and time-averaged manner. This is due to the thermal energy of the gas volume being finite and it takes more than just one pulse to substantially change its temperature or density distribution. As such, the actual attenuation received by any given pulse becomes a function of what came before, and for all intents and purposes is unpredictable The user must then rely on a pulse energy monitor downstream of the attenuator for more precise pulse energy information. A potential pitfall also exists for this mitigation strategy, since certainly in the case of soft X-rays the pulse energy monitor will be gas based as well and the very same filamentation effect is expected to impact the performance and precision of the energy measurement.

The results obtained in this study are predicated on the many assumptions being valid, such as the time scale of the pressure equilibration, and that thermal diffusion becomes the predominant mechanism for energy dissipation. There are of course other channels for the absorbed energy to escape the interaction volume perhaps at faster time scales and in a more efficient manner. Further studies to understand the

hydrodynamic and plasma-physics issues at shorter time scales of $< 1 \ \mu s$ are currently being carried out to validate these thermodynamic simulations. However, the fundamental issue with using a low-temperature or cold gas medium for attenuation or energy measurement stems from the fact that the total energy of the gas particles in the kinetic degrees of freedom is too low compared to the amount of energy it is designed to absorb for either attenuation or energy measurement purposes. Under typical operating conditions, the total kinetic energy of all gas molecules ($\sim NkT \sim PV$) in the entire volume in the beam path is often well below 1 mJ, which is roughly the average energy of the FEL pulses. On the inter-pulse time scale of 10 μ s for a high repetition rate FEL beam of 100 kHz, the thermal diffusivity of the gas is sufficiently low such that the diffusion length is of order 1 μ m and the absorbed energy stays relatively close to the beam, and does not move sufficiently far. Thus the gas heats up and expands, lowering its density, which in turn will change the amount of attenuation for the trailing pulses.

Unless the absorbed energy is dissipated sufficiently quickly, or the energy scale of the attenuator system itself is substantially higher than the energy of the FEL beam, its performance will be impacted. The possible mitigation mechanisms to minimize the filamentation effect must address either the dissipation speed and/or energy scale aspect. The size of the pipe could be optimized to allow more efficient cooling of the gas, and a longer gas volume would help as well by increasing the thermal contact of the gas volume with the cooling surfaces. To address the fundamental issue with the gas-based attenuator having too low an energy scale, one may envision a plasma-based attenuator system9 whose energy scale is much higher at a few eV or 10000 K. The operating power of a self-sustained plasma column can run as high as tens of kilowatts, much higher than the 200 W FEL power it would have to dissipate, thus the input FEL power becomes a perturbation to the plasma system, which is an entirely different situation in the current (cold) gas-based attenuator concept.

ACKNOWLEDEMENT

Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515. The authors acknowledge fruitful discussions with Bob Nagler, Alan Fisher, Philipp Sperling, Eric Galtier, and Mike Hogan.

REFERENCES

^[1] Cheng, Y.-H., Wahlstrand, J. K., Jhajj, N. & Milchberg, H. M., "The effect of long timescale gas dynamics on

femtosecond filamentation," Optics Express 21, 4740 (2013).

^[2] Schafer, D. W., "LCLS-II Gas Attenuator Design," unpublished (2015).

^[3] Feng, Y., Krzywinski, J., Schafer, D. W., Ortiz, E., Rowen, M., & Raubenheimer, T. O., "Filamentation Effect in a Gas Attenuator for High Repetition Rate X-ray FEL's," submitted to J. Synch. Rad. (2015).

^[4] Young, L., et al., "Femtosecond electronic response of atoms to ultra-intense X-rays," Nature 466, 56

^[4] Young, L., et al., Femtosecond electronic response of atoms to ultra-intense X-rays, Nature 466, 56 (2010).

^[5] Hoener, M., et al., "Ultraintense X-ray induced ionization, dissociation, and frustrated absorption in molecular nitrogen," Phys. Rev. Lett. 104, 253002 (2010).

^[6] Kondratenko, A. M. & Saldin, E. L., "Generation of coherent radiation by a relativistic electron beam in an undulator," Sov. Phys. Dokl. 24, 986 (1979).

^[7] Bonifacio, R., Pellegrini, C., and Narducci, L. M., "Collective instabilities and high-gain regime in a free electron laser," Opt. Comm. 50(6), 373 (1984).

^[8] Tiedtke, K., et al., "Gas detectors for X-ray lasers," J. Appl. Phys. 103, 094511 (2008).

^[9] Hershcovitch, A., Feng, Y., Fisher, A., Krzywinski, J., & Benwell, A., "A Plasma Attenuator for X-ray FEL's," unpublished (2015).