Short-pulse limits in optical instrumentation design for the SLAC Linac Coherent Light Source (LCLS)

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Abstract. The source properties of linac-driven X-Ray Free-Electron Lasers (XRFELs) operating in the Self-Amplified Spontaneous Emission (SASE) regime differ markedly from those of ordinary insertion devices on synchrotron storage rings. In the case of the 1.5 Å SLAC Linac Coherent Light Source (LCLS), the longitudinal output profile typically consists of a randomly-distributed train of fully-transversely-coherent micropulses of randomly varying intensity and an average length (corresponding to the source coherence length) two to three orders of magnitude smaller than the transverse diameter of the beam. Total pulse lengths are typically of the same order of size as the beam diameter. Both of these properties can be shown to significantly impact the performance of otherwise conventional synchrotron radiation optics; viz., mirrors, lenses, zone plates, crystals, multilayers, etc. In this paper we outline an analysis of short-pulse effects on selected optical components for the SLAC LCLS and discuss the implications for critical applications such as microfocusing and monochromatization.

1. INTRODUCTION

Past theoretical and experimental investigations of short pulse effects have frequently been motivated by the appearance of practical sources with temporal and spectral parameters falling outside ranges usually associated with conventional optical theory or experiment [1]. In recent decades, for example, the development of IR/visible/UV sources with pulse lengths extending down to the few-femtosecond range have stimulated the systematic re-investigation of the performance the performance of many types of optical elements and instruments, including mirrors, multilayers, diffraction gratings, refractive lenses, monochromators, and interferometers [2-10]. More recently, the advent of high power laser techniques for generating ultra-short X-ray pulses from plasmas [11], along with the continuing study and design development of a novel source of even shorter ultra-intense X-ray pulses, the X-Ray Free Electron Laser (XRFEL) [12], have stimulated a number of exploratory short-pulse investigations extending into the X-ray range [13,14,15]. In recent years, design studies for two practical XRFEL facilities operating in the Self Amplified Spontaneous Emission (SASE) mode [16,17], the TESLA FEL [18] and the SLAC Linac Coherent Light Source (LCLS) [19] have been completed and R&D toward their ultimate construction is currently in progress. In view of these developments, our goal in the present paper will be to assess the systematic extension of short-pulse analyses to the parameter range of these novel sources.

Our basic perspective will be to view the pulse parameter space of the SASE

XRFEL as a limiting case of the pulse parameters typically found on synchrotron storage rings. To initiate our discussion, we first recall the basic phase space properties predicted for the 1.5 Å SLAC LCLS [20,21]. In practical terms, the pulse is about as long as it is wide and has a temporal fine structure consisting of regions longitudinally on the order of 1 fs in length and transversely fully coherent (viz., with diameters equal to the full pulse diameter). The intensities of these regions, as well as their positions within the bunch, are random variables with statistics determined by the SASE gain process [21]. A set of 1.5 Å LCLS pulse dimensions contrasted with typical storage ring bunch parameters is listed in Table 1. It is evident that the LCLS pulse (in the lab frame) can be roughly characterized as having an aspect ratio of ~ 1 in all three planes, viz., a **"beginning," an "end," but no dominant "middle."**

TABLE 1. LCLS vs. storage ring radiation pulse dimensions.

Bunch Dimension	Storage Ring	LCLS
H [m]	50 - 250	~100
W [m]	150 - 1000	~100
L [m]	>10000	~100
L_m* [m]	N/A**	~0.3

*spatio-temporal fine structure parameter; **Gaussian density distribution

In designing optics for LCLS diagnostics and experimental applications it turns out that the preservation of not only the spectral-angular, but also the spatio-temporal distributions can be of significant importance. For example, for certain non-linear experiments that will require strong focusing of the LCLS beam to attain the requisite field strengths, it is assumed that the "microbunch" structure of the photon beam will be preserved [22], indeed, that it will be an essential factor in attaining the highest possible fields. Unfortunately, as will be outlined below, these same spatio-temporal parameters can inhibit, or even prevent, the preservation of uniform phase-space scaling. In the spectral-angular domain, this can also drastically impact the performance of instrumentation conventionally employed in the processing of typical X-ray pulses from conventional storage rings.

3. SHORT-PULSE INTERACTIONS WITH OPTICAL ELEMENTS

In a systematic assessment of short-pulse effects on the design and performance of optical elements and instrumentation, it is necessary to first consider the interaction of such pulses with matter. In this regard it useful to classify the interactions into convenient categories. For example, in terms of ascending time constants it is useful to distinguish among various types of scattering (both elastic and inelastic), viz.: Thompson, Rayleigh, Compton, atomic resonant, nuclear resonant, fluorescence, etc [23]. Another example would be a classification on the basis of field strength, viz., which leading terms need to be retained in the expansion of the polarization tensor in powers of the field intensity [24]. A third classification, of particular relevance to LCLS X-ray optics, is according to the scattering orders that need to be included for a particular material or optical element, viz., whether one must utilize a self-consistent field approach (dynamic scattering) or can approximate the interaction with a kinematic formalism. An illustration of the importance of this last distinction is shown in Fig. 1. In the kinematic approximation a wavefront can become short enough to suppress the Bragg diffraction; however, if higher-order scattering terms are incorporated, interference can still be generated along the Bragg direction even though such contributions will grow rapidly weaker. Although the small-scale features of LCLS pulses are still orders of magnitude longer than this limit (i.e., with respect to interatomic distances in crystals), diffraction performance can, in general, still be appreciably influenced if the dimensions of the scattering area are of the same order of size as the features of incoming X-ray pulse [13]. **In low-Z crystals [25] and multilayers this condition can hold both for the entire LCLS pulse as well as for its femtosecond features**.

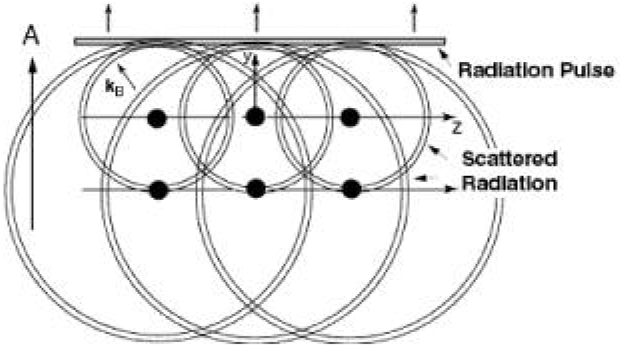

FIGURE 1. Schematic depiction of the limiting effect of temporal pulse length reduction on diffraction in a crystal. In the kinematic approximation, the pulse (A) can become short enough to inhibit interference along a given Bragg direction (denoted by $\mathbf{k}_B$).

4. SELECTED SCATTERING INTERACTIONS

4.1. Propagation through Dispersive Media

A 1-D formalism for the self-consistent propagation of ultrashort pulses through matter can be readily derived [1]. For initially Gaussian pulses both a gradual dilation of the pulse length and the evolution of a correlated phase are predicted. [1,26,27]. In conjunction with chirping of the LCLS electron beam, this can be used to control the length of the LCLS photon pulses in passage through media whose response is approximable by the analytical model.

4.2. Specular reflection:

The same formalism can also be used to calculate the response of specular optical elements (e.g., mirrors (single-reflection or multilayer) to ultra-short pulses. Due to the varying propagation of the spectral components comprising the pulse into the mirror material (determined by the boundary conditions satisfying each spectral component), variations in both the pulse length and phase distribution can be generated.

4.3. Diffraction

Scattering off a grating or crystal can strongly distort the spatio-temporal (as well as spectral-angular) phase-space profiles of the diffracted pulse. A simple analysis [14] yields the following estimates for temporal length (δ_i) and resolving power (R);

$$d \to d_1 \approx \frac{\ell}{\cos q_1}(\sin q_i - \sin q_1) \qquad \text{(temporal length dilation)} \qquad (2)$$

$$\frac{R}{R_{long\ \ pulse}} \to \frac{d}{d_1} \qquad \text{(Resolving Power reduction)} \qquad (3)$$

A more systematic analysis based on physical optics formalisms [28] can be applied to quantitatively assess the short-pulse performance of optical elements or instruments utilizing more than one grating (or crystal) [10]. In the X-ray range, the effects of absorption can also influence the performance of optics operating in transmission.

4.4. Refraction

For refraction, the distortion of a short optical pulse is governed not only by group and phase velocity dlfferences, i.e., by the optical constants of the material, but by the geometrical details of an optic's geometry [1]. For the LCLS, this has particular relevance to the design and performance of microfocusing optics, and will be discussed in more detail in the following section.

5. APPLICATIONS: MICROFOCUSING

A list of focusing methods under study for the LCLS is listed in Table 3. In the long-pulse limit relations between the transverse source size $s_{(LCLS)}$, distance from source to the optic (r), optical aperture ($d_{(LCLS)}$), and wavelength (λ), are easily derived. For a diffraction-limited source, we obtain

$$\sqrt{\left(lr\ /\ s_{(LCLS)}\right)^2 + s_{(LCLS)}{}^2} \cong d_{(LCLS)}.$$

TABLE 3. Selected categories of focusing and their characteristic angles of operation in the X-Ray range.

X-Ray Focusing Categories	**Typical X-Ray Incidence Angle**[a]
Specular ("Mirrors[b]")	θ_i~0 ("grazing incidence")
Reflective Diffractive ("Bragg-Fresnel Optics[c]")	θ_i<1
Transmissive Diffractive (Zone Plate w. >1 zone; "zone plate[d] ")	θ_i~π/2 ("normal incidence")
Transmissive Refractive (Zone Plate w. 1 zone; "refractive lens[e]")	θ_i~π/2 ("normal incidence")

[a]angle between the axis of the incoming light and the optical surface; [b]see, e.g., Ref. [29]; [c]see, e.g., Ref. [30]; [d]see, e.g., Ref. [31]; [e]see, e.g., Ref. [32]

In the case of the LCLS, {$s_{(LCLS)}$~100μ; r~50m; λ~1.5Å} => $d_{(LCLS)}$≅ 125μ. Thus, for focus to an mλ waist, λf/$d_{(LCLS)}$=mλ => f=m$d_{(LCLS)}$. E.g., for m=1, θ~π/4, f~$d_{(LCLS)}$. This relation applies to all the focusing categories listed in Table 3.

In the short pulse limit, the above relations can be substantially affected. Here we restrict ourselves to a discussion of normal-incidence optics, For passage through a refractive medium, expressions for the phase and group velocities [33] of an ultra-thin pulse are straightforwardly derived. Referring to Fig. 2, these are:

$$u_p = c[1 - d]^{-1} \quad (> c); \qquad u_g = c\left[n + l_0\left(\frac{d\,d}{d\,l}\right)_{l_0}\right]^{-1} \quad (< c),$$

where $\hat{n}$ $(= (1 - d) + \mathrm{ik})$ is the material's complex index of refraction. For k<<δ (as will be true for all passive low-Z optics in the LCLS wavelength range), the group velocity simplifies to:

$$\lambda_0\left(\frac{d\delta}{d\lambda}\right)_{\lambda_0} = \delta(2+S_\lambda^{f1}) \cong 2\delta \qquad \to \qquad u_g \cong c\left[1+\delta\right]^{1};$$

where $S_\lambda^{f1} = (\lambda/f1)(\partial f1/\partial\lambda)$, the sensitivity of f1 (the atomic phase scattering factor) to λ, is typically <<1 in regions away from absorption edges. The net result is that a temporal delay will develop between the contours of constant intensity (isophotes) and constant phase (isophases), affecting the size of the diffraction-limited focus attainable by elements such as refractive lenses and zone plates. We also note that, even in the absence of this differential delay, the temporal profile of an ultrashort pulse that is focused at too sharp an angle will be strongly distorted due to the substantially different lengths that the focused light must take from the outer edge of the optic in comparison to the central path.

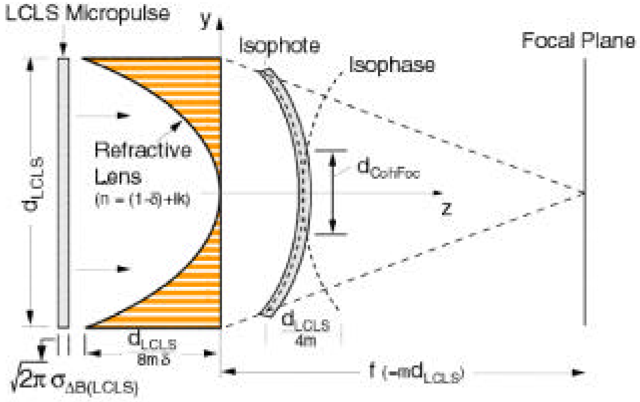

FIGURE 2. Schematic layout of refractive lens focusing an ultrashort LCLS pulse segment.

In the refractive lens the breakup of the wavefront into "zones" in which the isophase and isophote contours intersect is characterized by the parameter d_{CohFoc}, which is approximable by the expression $((2\pi)^{0.5} m d_{LCLS}\sigma_{\Delta B(LCLS)})^{0.5}$. This breakup will increase the diffraction-limited size of the beam at any value of m according to

$$m\lambda \to \lambda\sqrt{m^2 + \frac{m\,d_{LCLS}}{\sqrt{2\pi}\,\sigma_{\Delta B(LCLS)}}}\ .$$

We observe that as $(2\pi)^{0.5}\sigma_{\Delta B(LCLS)} \to\ >> d_{LCLS}$ (storage ring case), the focal waist converges to the ideal value mλ.

The temporal distortion (dilation) of the micro-features of the LCLS pulse will vary according to

$$\frac{\sqrt{2\pi}\,\sigma_{\Delta B(LCLS)}}{c} \to \frac{\sqrt{2\pi}\,\sigma_{\Delta B(LCLS)}}{c} + \frac{d_{LCLS}}{2c}\left(\sqrt{1+4m^2}+\frac{1}{4m}-2m\right)$$

for the refractive lens, and according to

$$\frac{\sqrt{2\pi}\,\sigma_{\Delta B(LCLS)}}{c} \to \frac{\sqrt{2\pi}\,\sigma_{\Delta B(LCLS)}}{c} + \frac{d_{LCLS}}{2c}\left(\sqrt{1+4m^2}-2m\right)$$

for a zone plate [15]. A set of representative values of these effects is given in Table 4.

TABLE 4. Selected LCLS short-pulse effects on the focusing performance of refractive lenses and zone plates at l=1.5 Å.

	Refractive lens (single zone)	**Zone Plate**
Ideal (diffraction-limited) focal waist at m=1	1.5 Å	1.5 Å
Actual focal waist at m=1	16.5 Å	16.5 Å
Unfocused micropulse length	2 fs	2 fs
Focused micropulse length (at m=1)	85 fs	43 fs

We can reiterate here that aberrations of this type occur at the leading and trailing edges of all synchrotron radiation pulses; the basic distinction between the LCLS and a conventional storage ring is that pulses at conventional storage rings are long enough so that these effects can usually be disregarded.

7. SUMMARY

We can summarize the basic results of our investigation as follows: 1) with regard to diffraction-limited performance strongly dispersive optics will tend to be ineffective over the leading and trailing edges of the full LCLS pulse - more than half the pulse energy could easily be excluded from the target phase space volume; 2) strongly dispersive optics (vs. frequency or angle) will also tend to convolve out the femtosecond temporal structure of the LCLS pulses: 3) to preserve the LCLS spatio-temporal structure optics with weak dispersion ($dq / df, \; dk / df \ll (L_m l / cd_{LCLS})$), e.g., relatively coarse-featured microstructures, should be used; 4) although specially-contoured mirrors (e.g., multilayer-coated ellipsoids) could be used to focus with minimal temporal distortion, trade-offs with dispersion in the other phase-space parameters will usually be involved (for example, although the isochrones and isophases along an ellipsoid's focus-to-focus trajectories coincide, there is a corresponding maximum dispersion in magnification along the longitudinal direction); 5) compound optical elements or configurations could possibly be developed to minimize or cancel certain types of distortion in selected phase-space regimes; 6) if substantial energy attenuation is tolerable, straightforward techniques (e.g., pinholes) could be developed for minimizing short-pulse effects by increasing beam divergence or by "slicing" out reduced cross sections of the LCLS photon pulse; 7) the development of a low-loss beam length dilator (to minimize the relative importance of edge effects without discarding most of the pulse photons) would be desirable.

We can conclude our discussion by noting that a general analytical treatment of short-pulse effects and their incorporation into phase-space transport through, and design of, optical elements is still lacking. For example, although in the present work we conducted our assessments of short-pulse effects primarily in spatio-temporal terms, an equivalent discussion could have been carried out equally well in the spectral-angular domain. Existing physical-optics-based treatments of radiation interacting with optical elements tend to formulate their analyses using superpositions of plane waves [34,35]; a more appropriate approach might be to include the temporal dependence explicitly [36,37] into the basis functions utilized in formulating the integrals of quasi-monochromatic propagation theory [28,38,39]. In view of the high field strengths generated by LCLS pulses, as well as to their full transverse coherence, formalisms of this type. should also be developed with the aim of adequately describing the self-consistent propagation of fields through matter. For example, theories that describe the propagation of fields through distorted matter (e.g., Ref. [40]) could in principle be integrated in an iterative fashion into a propagating-pulse formalism describing field or intensity-induced distortions of both the structural and optical properties of a medium in real time.

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