Proposal to generate 10 TW level femtosecond x-ray pulses from a baseline undulator in conventional SASE regime at the European XFEL

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Abstract

Output characteristics of the European XFEL have been previously studied assuming an operation point at 5 kA peak current. In this paper we explore the possibility to go well beyond such nominal peak current level. In order to illustrate the potential of the European XFEL accelerator complex we consider a bunch with 0.25 nC charge, compressed up to a peak current of 45 kA. An advantage of operating at such high peak current is the increase of the x-ray output peak power without any modification to the baseline design. Based on start-to-end simulations, we demonstrate that such high peak current, combined with undulator tapering, allows one to achieve up to a 100-fold increase in a peak power in the conventional SASE regime, compared to the nominal mode of operation. In particular, we find that 10 TW-power level, femtosecond x-ray pulses can be generated in the photon energy range between 3 keV and 5 keV, which is optimal for single biomolecule imaging. Our simulations are based on the exploitation of all the 21 cells foreseen for the SASE3 undulator beamline, and indicate that one can achieve diffraction to the desired resolution with 15 mJ (corresponding to about $3 \cdot 10^{13}$ photons) in pulses of about 3 fs, in the case of a 100 nm focus at the photon energy of 3.5 keV.

1 Introduction

Imaging of single molecules at atomic resolution using radiation from the European XFEL facility would enable a significant advance in structural biology, because it would provide means to obtain structural information

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of large macromolecular assemblies that cannot crystallize, for example membrane proteins. The imaging method "diffraction before destruction" [1]-[5] requires pulses containing enough photons to produce measurable diffraction patterns, and short enough to outrun radiation damage. The highest signals are achieved at the longest wavelength that supports a given resolution, which should be better than 0.3 nm. These considerations suggest that the ideal energy range for single biomolecule imaging spans between 3 keV and 5 keV [6]. The key metric for optimizing a photon source for single biomolecule imaging is the peak power. Ideally, the peak power should be of the order of 10 TW [7].

The baseline SASE undulator sources at the European XFEL will saturate at about 50 GW [8]. While this limit is very far from the 10 TW-level required for imaging single biomolecules, a proposal exists to improve the output power at the European XFEL by combining self-seeding [9]-[28], emittance spoiler foil [29]-[31], and undulator tapering techniques [32]-[41]. However, the realization of such proposal requires installing additional hardware in the undulator system and in the bunch compressor [7]. Here we explore a simpler method to reach practically the same result without additional hardware. This solution is based on the advantages of the European XFEL accelerator complex, which allows one to go well beyond the nominal 5 kA peak current.

The generation of x-ray SASE pulses at the European XFEL using strongly compressed electron bunches has many advantages, primarily because of the very high peak power, and very short pulse duration that can be achieved in this way [42]. Considering the baseline configuration of the European XFEL [8], and based on start-to-end simulations, we demonstrate here that it is possible to achieve a 100-fold increase in peak power by strongly compressing electron bunches with nominal charge. In this way we show (see Section 2 for more details) that 10 TW power level, 3 fs-long pulses at photon energies around 4 keV can be achieved in the SASE regime. This example illustrates the potential for improving the performance of the European XFEL without additional hardware.

The solution to generate 10 TW power level proposed in this article is not without complexities. The price for using a very high peak-current is a large energy chirp within the electron bunch, yielding in its turn a large (about 1%) SASE radiation bandwidth. However, there are very important applications like bio-imaging, where such extra-pink x-ray beam is sufficiently monochromatic to be used as a source for experiments without further monochromatization.

The European XFEL features three x-ray sources. Three long undulators, operated in the SASE mode, will provide x-ray radiation in the photon energies between 0.26 keV and 25 keV. In order to enable high focus efficiency with commercially available mirrors (80 cm-long) at photon energies around 4 keV, the undulator source needs to be located as close as possible to the bio-imaging instrument. With this in mind we performed simulations for the baseline SASE3 undulator at a nominal electron beam energy of 17.5 GeV. We optimized our setup based on start-to-end simulations for an electron beam with 0.25 nC charge, compressed up to 45 kA peak current [43]. In this way, the SASE saturation power could be increased to about 0.5 TW.

In order to generate high-power x-ray pulses we exploit undulator tapering. Tapering consists in a slow reduction of the field strength of the undulator in order to preserve the resonance wavelength, while the kinetic energy of the electrons decreases due to the FEL process. The undulator taper can be simply implemented as discrete steps from one undulator segment to the next, by changing the undulator gap. In this way, the output power of the SASE3 undulator could be increased from the value of 0.5 TW in the SASE saturation regime to about 5 TW. The SASE3 undulator with 21 cells consists of two parts. The first is composed by an uniform undulator, the second consists of a tapered undulator. The SASE signal is exponentially amplified passing through the first uniform part. This is long enough, 9 cells, in order to reach saturation, which yields about 0.5 TW power. Finally, in the second part of the undulator the SASE output is enhanced up to 5 TW by taking advantage of magnetic field tapering over the last 12 cells.

From all applications of XFELs for life sciences, the main expectation and the main challenge is the determination of 3D structures of biomolecules and their complexes from diffraction images of single particles. Parameters of the accelerator complex and availability of long baseline undulators at the European XFEL offer the opportunity to build a beamline suitable for single biomolecular imaging experiments from the very beginning of the operation phase. In the next decade, no other infrastructure will offer such high peak current (up to about 50 kA) and high electron beam energy (up to about 17.5 GeV) enabling 10 TW mode of operation in the simplest SASE regime.

2 FEL Studies

In this section we present a feasibility study of the setup described above with the help of the FEL code Genesis 1.3 [44] running on a parallel machine. Results are presented for the SASE3 FEL line of the European XFEL, based on a statistical analysis consisting of 100 runs. The overall beam parameters used in the simulations are presented in Table 1.

Table 1
Parameters for the mode of operation at the European XFEL used in this paper.

	Units	
Undulator period	mm	68
Periods per cell	-	73
Total number of cells	-	21
Intersection length	m	1.1
Energy	GeV	17.5
Charge	nC	0.25

The beam parameters at the entrance of the SASE3 undulator, and the resistive wake inside the undulator are shown in Fig. 1, [43]. Full tracking calculations were used to find a new set of electron bunch parameters at the entrance of baseline undulators. The main effects influencing the electron beam acceleration and transport, such as space charge force, rf wakefields and coherent synchrotron radiation (CSR) effects inside magnetic compressors have been included. Our calculations account for both wakes and quantum fluctuations in the SASE1 undulator.

Using a bunch with larger slice emittance and energy spread, but also higher peak current, does not necessarily complicates reaching SASE saturation, because the increased peak current eases the effects of the increased longitudinal velocity spread. For example, the final normqlized slice emittance in the 45 kA case studied here is about 4 μm, but the SASE saturation length is in the very safe range of 9 undulator cells at photon energies around 4 keV. The extreme working point at 45 kA peak current is very interesting, because the radiation peak power at saturation is ten-fold increased up to about 0.5 TW. The problem with operation at higher peak current is that wake fields become larger and, therefore, the energy chirp within the electron bunch becomes in its turn more and more important. In our case of interest, the variation in the electron energy within the bunch can be large compared to the Pierce parameter ρ (i.e. with the slice gain-bandwidth) [43], but this does not result in gain reduction [2]. Specifically, simulations show that the large energy chirp along the electron bunch only yields a large (about 1%) output radiation bandwidth.

Due to collective effects in the bunch compression system, emittances in the horizontal and vertical directions are significantly different. As a result, the electron beam looks highly asymmetric in the transverse plane: in the

[2] In order to incur in gain reduction, one should have a relative variation in the electron beam energy comparable or larger than the Pierce parameter ρ within a cooperation length.

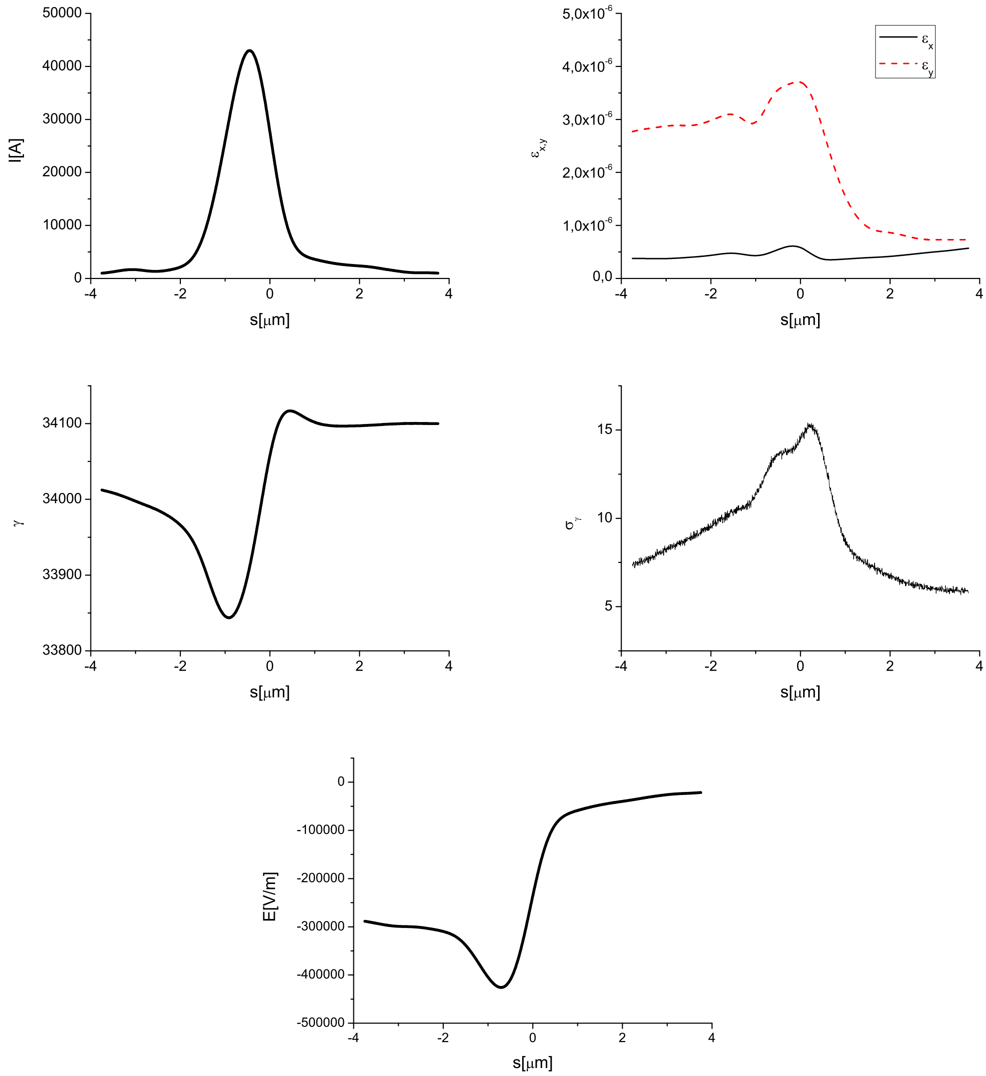

Fig. 1. Results from electron beam start-to-end simulations at the entrance of SASE3. (First Row, Left) Current profile. (First Row, Right) Normalized emittance as a function of the position inside the electron beam. (Second Row, Left) Energy profile along the beam. (Second Row, Right) Electron beam energy spread profile. (Bottom row) Resistive wakefields in the SASE3 undulator.

horizontal direction $\sigma_x \sim 20\mu$m, while in the vertical direction $\sigma_y \sim 50\mu$m. The evolution of the transverse electron bunch dimensions are plotted in Fig. 2. The evolution of the transverse electron bunch dimensions is plotted in Fig. 2, and the correspondent quadrupole strength is shown in Fig. 3. The undulator is tapered according to the law in Fig. 4. The quadrupole strength and the tapering have been optimized to maximize the final output power.

The output characteristics, in terms of power and spectrum, are plotted in Fig. 5. Inspection of the plots shows that one can reach 5 TW pulses with a bandwidth of about 1%. Fig. 6 shows the distribution of the radiation

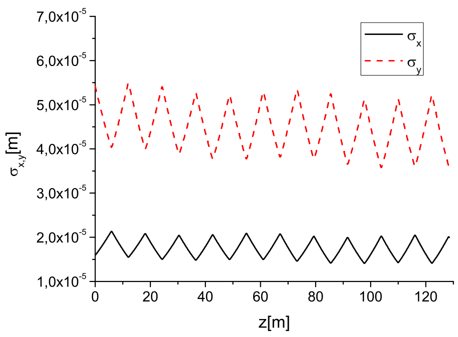

Fig. 2. Evolution of the horizontal and vertical dimensions of the electron bunch as a function of the distance inside the SASE3 undulator. The plots refer to the longitudinal position inside the bunch corresponding to the maximum current value.

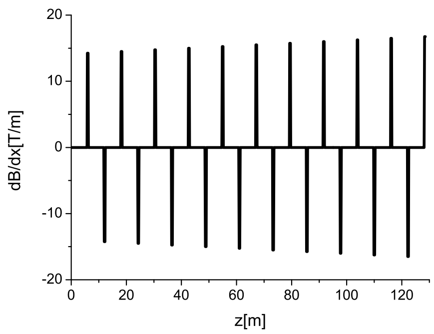

Fig. 3. Quadrupole strength along the undulator.

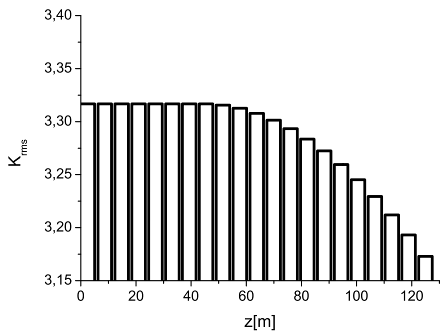

Fig. 4. Tapering law.

pulse energy per unit surface and angular distribution of the exit of the setup. Finally, in Fig. 7 we plot the evolution of the output energy in the photon pulse and of the variance of the energy fluctuation as a function of the distance inside the output undulator.

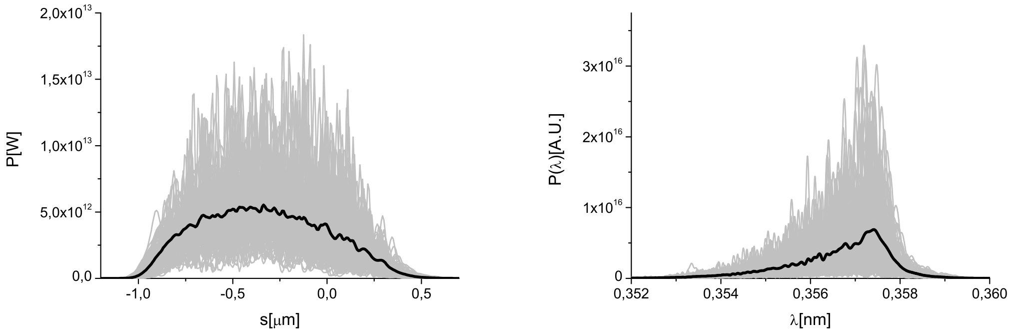

Fig. 5. Power and spectrum produced in the SASE mode at saturation with undulator tapering. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

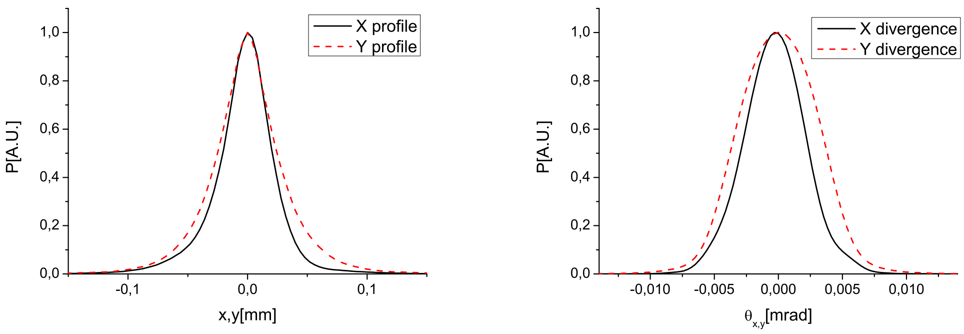

Fig. 6. Distribution of the radiation pulse energy per unit surface and angular distribution of the exit of the setup.

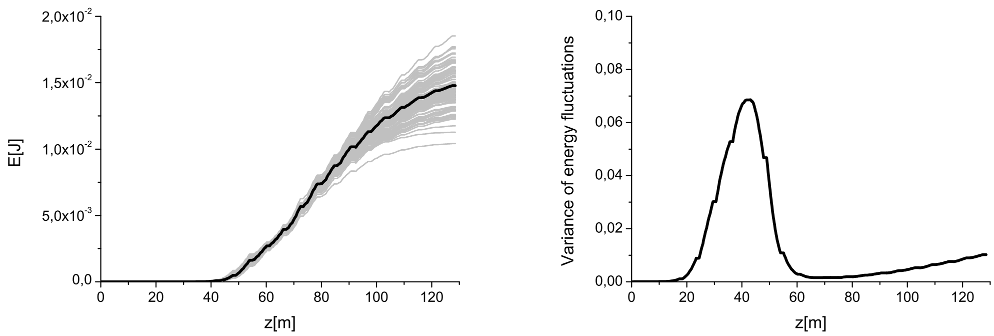

Fig. 7. Evolution of the output energy in the photon pulse and of the variance of the energy fluctuation as a function of the distance inside the output undulator, with tapering. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

3 Conclusions

The nominal design parameters for the European XFEL for a 0.25 nC electron bunch, which allow for SASE saturation with 0.4 μm normalized slice emittance and 5 kA peak current are described in [45]. In this article we note that the European XFEL accelerator complex is flexible enough to be reconfigured for much higher bunch peak-current. In this case, the new beam parameters are simply set in the control room, and do not require hardware modifications in the tunnel. This flexibility is demonstrated by studying the new acceleration and compression parameters required over a wide range of a peak current values well beyond the nominal 5 kA [43]. For each case, full tracking calculations were used to find a new set of electron bunch parameters at the entrance of baseline undulators. The main effects influencing the electron beam acceleration and transport, such as space charge force, rf wakefields and coherent synchrotron radiation (CSR) effects inside magnetic compressors have been included. Using a bunch with larger slice emittance and energy spread, but also higher peak current, does not necessarily complicates reaching SASE saturation, because the increased peak current eases the effects of the increased longitudinal velocity spread. For example, the final slice normalized emittance in the 45 kA case studied here is about 4 μm, but the SASE saturation length is in very safe range of 9 undulator cells at photon energies around 4 keV. The extreme working point at 45 kA peak current is very interesting, because the radiation peak power at saturation is ten-fold increased up to about 0.5 TW. The problem with operation at higher peak current is that wake fields become larger and, therefore, the energy chirp within the electron bunch becomes in its turn more and more important. In our case of interest, the variation in the electron energy within bunch can be large compared to the Pierce parameter ρ (i.e. with the slice gain-bandwidth) [43], but this does not result in gain reduction. Specifically, simulations show that the large energy chirp along the electron bunch only yields a large (about 1%) output radiation bandwidth.

For certain experiments, a high degree of monochromacity is not needed. An important class of experiments when a large radiation bandwidth is not detrimental is single biomolecular imaging. In such instances, photon fluence rather than spectral photon density is a premium. One obvious way to enhance the SASE efficiency is by properly configuring undulators with variable gap. It has been shown that this approach allows one to increase the peak power to 5 TW by taking advantage of an undulator magnetic-field taper over the baseline SASE3 undulator. Such unique feature will be available only at the European XFEL for a long time. In fact, the European XFEL uses a super-conducting L-band linac to accelerate beams which can be compressed up to extremely high peak current (about 50 kA), with still a reasonable electron bunch quality. Moreover, high electron beam energy (up to about 17.5 GeV) and long undulators with high K values imply a high peak output-power.

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References

[1] J. Hajdu, Curr. Opin. Struct. Biol. 10, 569 (2000)
[2] R. Neutze et al., Nature 406, 752 (2000)
[3] H. Chapman et al., Nat. Phys. 2, p. 839 (2006).
[4] K. J. Gaffney and H. N. Chapman, Science 316, 1444 (2007)
[5] M. M. Seibert et al., Nature 470 (7332) 78-81 (2011)
[6] S. Baradaran et al., LCLS-II New Instruments Workshops Report, SLAC-R-993 (2012), see Section 4.3.2. by H. Chapman et al., and Section 4.3.3. by F. R. N. C. Maia et al.
[7] S. Serkez et al., Proposal for a scheme to generate 10 TW-level femtosecond x-ray pulses for imaging single protein molecules at the European XFEL, DESY 13-101, http://arxiv.org/abs/1306.0804 (2013).
[8] Th. Tschentscher, "Layout of the x-Ray Systems at the European XFEL", Technical Report 10.3204/XFEL.EU/TR-2011-001 (2011).
[9] J. Feldhaus et al., Optics. Comm. 140, 341 (1997).
[10] E. Saldin, E. Schneidmiller, Yu. Shvyd'ko and M. Yurkov, NIM A 475 357 (2001).
[11] E. Saldin, E. Schneidmiller and M. Yurkov, NIM A 445 178 (2000).
[12] R. Treusch, W. Brefeld, J. Feldhaus and U Hahn, Ann. report 2001 "The seeding project for the FEL in TTF phase II" (2001).
[13] A. Marinelli et al., Comparison of HGHG and Self Seeded Scheme for the Production of Narrow Bandwidth FEL Radiation, Proceedings of FEL 2008, MOPPH009, Gyeongju (2008).
[14] G. Geloni, V. Kocharyan and E. Saldin, "Scheme for generation of highly monochromatic X-rays from a baseline XFEL undulator", DESY 10-033 (2010).
[15] Y. Ding, Z. Huang and R. Ruth, Phys.Rev.ST Accel.Beams, vol. 13, p. 060703 (2010).
[16] G. Geloni, V. Kocharyan and E. Saldin, "A simple method for controlling the line width of SASE X-ray FELs", DESY 10-053 (2010).
[17] G. Geloni, V. Kocharyan and E. Saldin, "A Cascade self-seeding scheme with wake monochromator for narrow-bandwidth X-ray FELs", DESY 10-080 (2010).
[18] Geloni, G., Kocharyan, V., and Saldin, E., "Cost-effective way to enhance the capabilities of the LCLS baseline", DESY 10-133 (2010).

[19] J. Wu et al., ”Staged self-seeding scheme for narrow bandwidth , ultra-short X-ray harmonic generation free electron laser at LCLS”, proceedings of 2010 FEL conference, Malmo, Sweden, (2010).
[20] Geloni, G., Kocharyan V., and Saldin, E., ”Generation of doublet spectral lines at self-seeded X-ray FELs”, DESY 10-199 (2010), and Optics Communications, 284, 13, 3348 (2011)
[21] Geloni, G., Kocharyan, V., and Saldin, E., ”Production of transform-limited X-ray pulses through self-seeding at the European X-ray FEL”, DESY 11-165 (2011).
[22] Geloni, G., Kocharyan V., and Saldin, E., ”A novel Self-seeding scheme for hard X-ray FELs”, Journal of Modern Optics, vol. 58, issue 16, pp. 1391-1403, DOI:10.1080/09500340.2011.586473 (2011)
[23] J. Wu et al., Simulation of the Hard X-ray Self-seeding FEL at LCLS, MOPB09, FEL 2011 Conference proceedings, Shanghai, China (2011).
[24] J. Amann et al., Nature Photonics, DOI: 10.1038/NPHOTON.2012.180 (2012).
[25] R. R. Lindberg and Yu.V. Shvydko, Phys. Rev. ST Accel. Beams 15, 100702 (2012).
[26] Y. Feng et al., ”System design for self-seeding the LCLS at soft X-ray energies”, Proceedings of the 24th International FEL Conference, Nara, Japan (2012).
[27] S. Serkez, G. Geloni, V. Kocharyan and E. Saldin, ”Grating monochromator for soft X-ray self-seeding the European XFEL”, DESY 13-040, http://arxiv.org/abs/1303.1392 (2013).
[28] G. Geloni, V. Kocharyan, E. Saldin, S. Serkez and M. Tolkiehn, ”Wake monochromator in asymmetric and symmetric Bragg and Laue geometry for self-seeding the European XFEL”, DESY 13-013 (2013).
[29] P. Emma, K. Bane, M. Cornacchia, Z. Huang, H. Schlarb, G. Stupakov, and D. Walz, PRL 92, 074801-1 (2004).
[30] P. Emma, M. Borland and Z. Huang, Proceedings of the FEL Conference 2004, TUBIS01, p.333 (2004).
[31] Y. Ding , et al., PRL 109, 254802-1 (2012).
[32] A. Lin and J.M. Dawson, Phys. Rev. Lett. 42 2172 (1986).
[33] P. Sprangle, C.M. Tang and W.M. Manheimer, Phys. Rev. Lett. 43 1932 (1979).
[34] N.M. Kroll, P. Morton and M.N. Rosenbluth, IEEE J. Quantum Electron., QE-17, 1436 (1981).
[35] T.J. Orzechovski et al., Phys. Rev. Lett. 57, 2172 (1986).
[36] W. Fawley et al., NIM A 483 p 537 (2002).
[37] M. Cornacchia et al., J. Synchrotron rad. 11, 227-238 (2004).
[38] X. Wang et al., PRL 103, 154801 (2009).
[39] G. Geloni, V. Kocharyan and E. Saldin, ”Scheme for generation of fully coherent, TW power level hard x-ray pulses from baseline undulators at the European XFEL”, DESY 10-108 (2010).
[40] W.M. Fawley et al., Toward TW-level LCLS radiation pulses, TUOA4,

FEL 2011 Conference proceedings, Shanghai, China (2011).
[41] Y. Jiao et al. Phys. Rev. ST Accel. Beams 15, 050704 (2012).
[42] T. Limberg et al., "Optimized bunch compressor system for the European XFEL", Proceedings of 2005 Particle Accelerator Conference, Knoxville, Tennessee, 1236, http://accelconf.web.cern.ch/AccelConf/P05/PAPERS/RPPT011.PDF (2005)
[43] I. Zagorodnov, "Compression scenarios for the European XFEL", http://www.desy.de/fel-beam/data/talks/files/Zagorodnov_ACC2012_ready_new.pptx, (2012).
[44] S. Reiche et al., Nucl. Instr. and Meth. A 429, 243 (1999).
[45] I. Zagorodnov, "Beam Dynamics Simulations for XFEL", http://www.desy.de/xfel-beam/s2e (2011).