Plasma surface dynamics and smoothing in the relativistic few-cycle regime

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Abstract. Efficient production of coherent harmonic radiation from solid targets relies critically on the formation of smooth, short density scalelength plasmas. Recent experimental results (Dromey et al 2009 Nat. Phys. 5 146) suggest, however, that the target roughness on the scale of the emitted harmonic wavelength does not result in diffuse reflection—in apparent contradiction to the Rayleigh criterion for coherent reflection. In this paper we show, for the first time, using analytic theory and 2D PIC simulations, that the interaction of relativistically strong laser pulses with corrugated target surfaces results in a highly effective smoothing of the interaction surface and consequently the generation of highly collimated and temporally confined XUV pulses from rough targets, in excellent agreement with experimental observations.

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The dynamics of the plasma–vacuum surface irradiated by intense laser pulses is of fundamental importance for understanding the laser–plasma interaction. It is also of critical importance for the harmonic radiation produced from such surfaces [1]–[4], which has recently been

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demonstrated experimentally to provide the basis for a bright source of diffraction-limited extreme ultraviolet (XUV) radiation [5] with attosecond structure in the temporal domain [6]. Such harmonic sources possess unique properties that make them highly attractive for future experiments seeking to address the fundamentals of electron dynamics in matter (see [7] and references therein) and for experimental challenges, such as reaching the Schwinger limit [8, 9].

One limit to the ultimate potential of such harmonics—particularly with respect to the extreme focusing suggested in [8]—is the role of any surface imperfections such as in terms of shape and roughness. These can greatly affect the generation process and the angular and temporal structures of the beam.

However, recent results of Dromey et al showed that the reflection of high-order harmonics from initially rough targets was consistent with the existence of a very effective smoothing mechanism rather than modulation growth due to instabilities [5, 10]. Motivated by this surprising behavior, we have investigated the interaction of a relativistically strong laser pulse with an overdense, modulated plasma surface. Here, we present for the first time the theoretical basis, both analytically and with particle-in-cell (PIC) simulations, for rapid smoothing of the plasma–vacuum interface and show it to be effective on length scales below the transverse electron oscillation amplitude.

To gain insights into the particle motion in the overdense plasma, we use a simple one-dimensional (1D) model [4], [11]–[14]. The analysis presented below is strictly applicable only for laser foci much larger than the excursion of the electrons, which is typically met for the discussed parameter range. This single-particle model describes the motion of an incompressible electron layer bound to immobile ion background via charge-separation fields under the influence of normally incident, linearly polarized electromagnetic wave. This layer, later referred to simply as the electron, is initially located on the vacuum–plasma interface at $x = 0$. Taking into account that the charge separation fields are proportional to the electron longitudinal coordinate $x$, the equations of motion can be readily obtained as

$$\frac{dp_x}{dt} = -\beta_y \frac{\partial a_y(t, x)}{\partial x} + n_e x,$$

$$\frac{dp_y}{dt} = \frac{\partial a_y(t, x)}{\partial t},$$

where $x$ and $y$ are the propagation and transversal coordinates, respectively; $\beta_x, y$ and $p_x, y$ are the velocity and momenta components, respectively; $a_y$ is the driving vector potential and $n_e$ is the electron density. We work in relativistic units. The normalized quantities for vector potential $a$, time $t$, length $l$, momentum $p$ and density $n$ are obtained from their counterparts in SI units $A, t', l', p'$ and $n'$ via

$$a = \frac{eA}{m_e c}, \quad t = \omega_L l', \quad l = \frac{\omega_L}{c} l', \quad p = \frac{p'}{m_e c}, \quad n = \frac{n'}{n_{cr}}.$$  

Here $e$ and $m_e$ are the charge and the mass of the electron, $\omega_L$ is the laser angular frequency, $c$ is the speed of light in vacuum and $n_{cr} = \varepsilon_0 m_e c^2/\varepsilon^2$ is the electron critical density.

In equations (2) $a_y(t, x)$ denotes the driving vector potential on the vacuum–plasma interface, which results from the interference between the incident and reflected waves. It can be found by imposing the standard boundary conditions for the continuity of electromagnetic fields, i.e. of the vector potential and its spatial derivative $\partial_x a_y$ at the plasma–vacuum interface. Without losing generality, the incident $a_i$, reflected $a_r$ and transmitted $a_t$ vector potentials
Figure 1. Electron motion obtained using the capacitor model for a laser pulse with $a_0 = 10$ with 4-cycle FWHM duration and $n_e = 400$. The electron is initially located at $x_e = y_e = 0$. Panel (a) shows the electron trajectory; panel (b) demonstrates the behavior of the transverse coordinate $y_e$ in time; in panel (c), the solid line represents the longitudinal coordinate $x_e$ of the electron (vertical axis) versus time (horizontal axis) obtained from the model; the color-coded image displays the spatio-temporal picture of the electron density obtained from 1D PIC simulations with the same laser and plasma parameters.

Figure 1 can be taken in the form $a'_i(t - x') = -E_i \cdot \sin(t - x')$, $a'_r(t + x') = -E_r \cdot \sin(t + x' + \phi)$, and $a'_t(t, x') = -E_t \cdot \sin(t + \phi) \cdot \exp[-\omega_p(x' - x)]$, respectively. With $x'$ we denote the longitudinal coordinate for the electromagnetic field, while keeping the notation of $x$ for the coordinate of the electron. Applying the boundary conditions (thus setting $x' = x$) one obtains $E_i = E_r = \frac{1}{2} \cdot \sqrt{1 + \omega_p^2} \cdot E_i$ and $\phi = 2\phi = 2(\alpha - x)$, where $\alpha \simeq \arctan \omega_p$ with $\omega_p = \sqrt{n_e}$ being the plasma frequency. One can use the transmitted vector potential at $x = x'$ to obtain the driving vector potential:

$$a_y = -\frac{2E_i}{\sqrt{1 + \omega_p^2}} \sin(t - x + \alpha) \cdot e^{-\omega_p(x' - x)}.$$  (4)

It is important to note that the actual vector potential driving the electron is approximately $\omega_p/2$ times lower than the incident one. As a consequence, relativistic effects on the electron motion and corresponding corrections to the skin depth become important only when the amplitude of the incoming light $a_0$ exceeds $\omega_p/2$ [11].

Results of the model calculations are presented in figure 1. The trajectory of an electron interacting with a laser pulse having a Gaussian envelope of 4-cycle full-width at half-maximum (FWHM) duration $\tau_{\text{FWHM}}$ and amplitude $a_0 = 10$ (corresponding to an intensity of $1.37 \times 10^{20}$ W cm$^{-2}$ for a laser wavelength of $\lambda_L = 1 \mu$m) is shown in figure 1(a). Plasma density is $n_e = 400$. Figure 1(b) shows the transverse coordinate $y$ as a function of time $t$. In figure 1(c) the solid line shows the longitudinal coordinate $x$ (the horizontal axis) as a function of time $t$ (the vertical axis).

Figure 1(c) allows us to understand the origin of the harmonic generation process. One can see that during the interaction the model-electron (the step-like reflecting surface) oscillates in
Figure 2. Dependence of the amplitudes of longitudinal $x_{\text{max}}$ (a) and transverse $y_{\text{max}}$ (b) motion on the laser amplitude $a_0$. In panel (a), the circles represent the results of 1D PIC simulations and the solid line shows the results of numerical integration of the capacitor model. In panel (b), the solid line depicts numerical integration of the model equations and the dashed line is obtained from equation (5).

The solid line in figure 2(a) shows the dependence of the longitudinal displacement of the electron layer on the laser amplitude $a_0$ obtained from the numerical integration of the model equations. It is worth stating that these results (and thus the value of the charge-separation field) coincide perfectly (for the case of total reflection) with the model based on the pressure balance and used in the analytical treatment of ion acceleration [17].

In this paper, we want to pay attention to the transverse motion of the electron, which extends to a considerable fraction of the laser wavelength (see figure 1(b)) and might therefore be responsible for the surface smoothing. Indeed, if the transverse motion of the electron exceeds the characteristic size of the modulations on a rough surface, then the roughness is likely to disappear.

In assessing the role of the transverse motion as a possible smoothing mechanism, a simple expression for its amplitude is needed. Neglecting longitudinal motion, one can obtain from equation (4) an estimate for the amplitude of the transverse motion $y_{\text{max}}$:

$$y_{\text{max}} \approx 2 \cdot a_0 \sqrt{\omega_p^2 + 4 \omega_0^2}. \tag{5}$$

The dependence of the transverse electron motion amplitude $y_{\text{max}}$ on the laser pulse amplitude $a_0$ for plasma density $n_e = 400$ is shown in figure 2(b). The solid line shows the results obtained by numerically solving the model equations and the dashed line represents equation (5). The simple estimate (5) works fairly well for the parameter range studied, and its simplicity makes it convenient for the following estimates. More accurate results can be obtained by numerically integrating the model equations.

Having estimated the amplitude of the transverse coordinate $y_{\text{max}}$, one can establish an ad hoc criterion for surface smoothing to occur based on the ratio of this amplitude to the characteristic roughness size $h$. For instance, where the transverse motion is of the order of
the characteristic roughness size within the interaction area, considerable smoothing can be expected. One can define a dimensionless parameter $\xi$ separating the case when smoothing takes place from the case when the roughness survives during the interaction:

$$
\xi = \frac{2a_0}{\sqrt{\omega_0^2 + 4a_0^2 \cdot h_y}} \cdot e^{-\omega_0 h_x},
$$

where $h_x$ and $h_y$ (we assume that if $h_x = 0$, then $h_y = 0$ and vice versa) are the characteristic roughness sizes in the longitudinal and transverse directions, respectively. We make an assumption that the boundary conditions stay the same independent of surface structure and that the field exponentially decays inside the plasma. In the case when $\xi \gg 1$, the roughness according to our criterion vanishes. We show further that even in the case when $\xi \sim 1$, substantial smoothing is observed.

To check the validity of the afore-described model and to demonstrate the surface smoothing, we have conducted a series of 1D and 2D PIC simulations using the code PICWIG [21] with clean and rough surfaces for different laser amplitudes $a_0$. The code allows the simulation of the interaction of intense laser pulses with pre-ionized non-collisional plasma with the beam incident normally on the target. The typical plasma density used in 1D simulations is $n_e = 400$ and $n_e = 30$ in the 2D case. A step-like vacuum–plasma interface is assumed, the ions are immobile. In the 2D case, the surface is almost always modulated sinusoidally in order to simulate the roughness (see the left part of figure 6). For convenience, the modulation period and amplitude are linked and the position of the vacuum–plasma interface is given by the law $x = h \cdot \sin(2\pi y / h)$. We have also performed runs with the random roughness by taking the superposition of ten sinusoidal functions with random amplitudes, frequencies and phases to check that the results are similar and do not depend on the exact structure of the surface. The laser pulse amplitude was varied up to $a_0 = 20$ in the 1D case and is fixed to $a_0 = 10$ in the 2D scenario. Throughout the paper we use FWHM of the electric field as the definition of the laser pulse duration and use pulses with an electric field that has a Gaussian envelope function in both time and space.

$$
E_y(t, x, y) = E_0 \cdot \exp \left[ -\frac{y^2}{2\rho^2} \right] \exp \left[ -\frac{(t-x)^2}{2\tau_L^2} \right],
$$

where $\rho$ and $\tau_L$ are the width of the focus and duration of the laser pulse, respectively. The FWHM duration is related to $\tau_L$ by $\tau_{FWHM} = \tau_L \sqrt{8 \ln 2}$. In the 1D case, the size of the simulation box is $7\lambda_L$, the time step is $T_L/1000$ with $T_L$ the period of the driving laser, the spatial grid size is $\lambda_L/1000$ and each plasma cell is initially occupied by 1000 macro-electrons. In the 2D case, the size of the simulation box is $3.5\lambda_L$ in the laser propagation direction and $40\lambda_L$ in the polarization direction. The time step is $T_L/300$ and the laser propagation direction spatial step is $\lambda_L/300$. Each cell is initially occupied by 50 macro-electrons.

The results of 1D simulations are presented in figures 1(c), 2(a) and 3. The color-coded image in figure 1(c) presents the spatio-temporal evolution of the electron density obtained from simulations with the same laser and plasma parameters as in the model (solid line). One can see that the model is in agreement with the PIC simulations. Figure 2(a) shows the results of the model calculations of longitudinal electron amplitude (solid line) for different laser amplitudes $a_0$ compared to simulations (circles). The fact that simulation results lie on the curve obtained from the model and as longitudinal motion is directly correlated to transverse motion allows us to claim that the model works well and gives correct estimates for both the longitudinal...
Figure 3. Longitudinal (a) and transverse (b) coordinates of the model electron (thick black line) and macro-electrons from PIC simulation (colored lines) versus time. Laser and target parameters are the same as in figure 1.

(figure 2(a)) and transverse (figure 2(b)) coordinates. The latter are hard to obtain from 1D PIC simulation as the particles leave the interaction region and are very intricate to trace. This can be seen in figure 3, where the longitudinal (a) and transverse (b) coordinates as functions of time for 100 macro-electrons obtained from the 1D PIC simulations (color lines) as well as...
Figure 4. Far-field distribution of the reflected harmonics beam $200\lambda_L$ away from the target for (a) a smooth surface, (b) a surface with modulation size $h = 0.05\lambda_L$, (c) a surface with modulation size $h = 0.1\lambda_L$ and (d) a surface with modulation size $h = 0.2\lambda_L$.

In the 2D case, we investigate the spatial beaming of harmonics as a possible indication of smoothing. We analyze the propagation of the harmonics emission away from the target using Kirchhoff diffraction theory [22] following the approach used in earlier investigations [9, 23]. The harmonic beam (from the 15th to the 25th harmonic, central wavelength $0.05\lambda_L$) $200\lambda_L$ away from the target is shown in figure 4. In all four panels of figure 4 the color surface presents the results of the model calculations (thick black lines) are shown. One can see that although the longitudinal motion of the macro-electrons in the PIC simulation is complex and particles leave the interaction region gaining energy from the laser, the motion of the reflecting layer can still be described by the simple model presented earlier. Figure 3(b) also illustrates the main disadvantage of the model—it does not take the absorption into consideration. The transverse amplitude of the particles in the PIC simulations is bigger than the amplitude of the model particle. One can see that the transverse coordinate of many electrons from the PIC simulations reaches a certain amplitude and then remains constant. Those are the particles that by absorbing a certain fraction of laser energy, shoot through the target and exit on its rear side. It is a known phenomenon and is described, for example, in [13], and in [18]–[20], where the electrons that exit on the rear side form the longitudinal field that accelerates the ions. This process is referred to as target normal sheath acceleration.
the distribution of normalized intensity of the filtered harmonics as a function of both time $t$ and the transverse coordinate $y$ (the ceiling panel shows the same data as a color-coded image). The upper right plane shows the projection of the beam to the time axis; thus the time structure of the harmonics beam exhibiting a train of several attosecond pulses. On the upper-left plane the intensity distribution of the harmonics beam as a function of transverse coordinate $y$ is shown (black solid line). The results presented in figures 4(a)–(d) are obtained for a surface with sinusoidal modulation with size $h = 0$ (smooth surface, $\xi \rightarrow \infty$), $h = 0.05\lambda_L$ ($\xi \approx 0.6$), $h = 0.1\lambda_L$ ($\xi \approx 0.05$) and $h = 0.2\lambda_L$ ($\xi \approx 0.0008$), respectively. The ripple wave number was chosen to be typical of the experiment. There are several important points to mention.

Firstly, for the simulation parameters considered the distance of $200\lambda_L$ corresponds to the position of the harmonics focus due to surface denting as discussed in the paper by Hörlein et al [9]. This can be illustrated from figure 4(a) by the fact that the transverse width of the reflected harmonics beam (see the graph in the upper left plane) is much less than the initial laser width with $\rho = 5\lambda_L$.

Secondly, for the dimensionless smoothing parameter $\xi$ of the order of unity, the spatial and temporal structures of the harmonic beam are not influenced by the surface roughness. Figure 4 shows the harmonic orders from the 15th to the 25th, which should undergo diffuse reflection by each of the rough surfaces simulated. Contrary to the Rayleigh criterion [24], but in agreement with experimental observation [5], almost no change in the harmonic beam structure is observed for $\xi \approx 0.6$ (figure 4(b)) in good agreement with our ad hoc smoothing criterion. Surfaces with $\xi \ll 1$ (figures 4(c) and (d)) lead to the speckle-like diffraction picture with more energy going to the wings of the beam. The fact that the beam is still tolerably collimated hints that even though $\xi \ll 1$, the characteristic surface roughness was significantly diminished during the interaction.

To check that the smoothing does not depend on the exact surface profile, we have performed simulations with random roughness profile obtained by the superposition of ten sinusoidal functions with random amplitudes, frequencies and phases. The part of the surface profile is presented in figure 5(a) and has the amplitude $h \approx 0.03\lambda_L$ in both the directions leading to the dimensionless smoothing parameter $\xi \approx 1.8$. The far-field distribution of the harmonic beam generated on the random roughness surface is presented in figure 5(b); the parameters

**Figure 5.** (a) Random roughness surface profile and (b) the far-field distribution of the harmonic beam generated on this target $200\lambda_L$ away.
of the figure are the same as for figure 4. One can see that the beam profile remains almost unaffected compared to figure 4(a).

The analysis of the spatial structure of harmonics generated on the corrugated surfaces exhibits collimated beam structure and serves as indirect proof of the surface smoothing.

Direct proof of the surface smoothing can be found in figure 6, where initial density distribution (as a function of the longitudinal and transverse coordinates) and the density distribution near the moment when the pulse maximum reaches the surface are shown (left and right panels, respectively). The results here are presented for the surface with $\xi \approx 0.6$. The evolution of the electron density in time can be traced in the animation made from simulation data (see the supplementary video, available at stacks.iop.org/NJP/13/023008/mmedia), showing that the transverse motion of the electrons leads to rapid (in contrast to the hydrodynamically slow smoothing due to ion motion) smoothing of the corrugation.

In conclusion, we have shown for the first time that surface smoothing of a rough target surface during the interaction of relativistically intense laser pulse can be sufficient to allow diffraction-limited beaming of harmonic radiation—contrary to the expectation based on the Rayleigh criterion. This effect does not rely on the slow smoothing due to ion motion and is a direct result of the large spatial amplitude of the electron trajectories in relativistic laser interactions. This finding has a direct impact on the peak intensities that can be achieved at shortest wavelengths and suggests that extremely high-quality keV harmonic beams are achievable. Moreover, it shows that in the discussed parameter range there can be a limitation to the recently proposed harmonic generation enhancement scheme using the gratings [25, 26] as the grating might not survive the interaction. The same probably holds for the question of the enhancement of absorption [14] on the corrugated surfaces. Both of these points are an interesting research topic as well as the interplay between the presented smoothing mechanism and the growth of instabilities for longer pulses. While the analysis presented here concentrates on normal incidence for simplicity and clarity, the results are clearly also valid for oblique incidence, where this effect was experimentally observed [5].

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