Production of proton beams with narrow-band energy spectra from laser-irradiated ultrathin foils

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Three-dimensional gridless particle simulations of proton acceleration via irradiation of a very thin foil by a short-pulse, high-intensity laser have been performed to evaluate recently proposed microstructured target configurations. It is found that a pure proton microdot target does not by itself result in a quasimonoenergetic proton beam. Such a beam can only be produced with a very lightly doped target, in qualitative agreement with one-dimensional theory. The simulations suggest that beam quality in current experiments could be dramatically improved by choosing microdot compositions with a 5–10 times lower proton fraction.

The emission of energetic ions from laser-produced plasmas is an established phenomenon that has been extensively studied over the past two decades. Since the advent of chirped pulse amplification lasers capable of achieving intensities in excess of 10^{20} W cm^{-2}, it has been possible to produce multi-MeV proton beams from irradiated foils [1–12]. Furthermore, in the past year it has been shown experimentally that proton or ion beams can be produced with a narrow range of energies [13–15]. It is these quasimonoenergetic beams that hold great promise for a range of applications, ranging from hadron therapy and pharmaceutical isotope production [16,17], to fast-ignition inertial confinement fusion [18,19].

It has also been shown recently that, when a higher contrast ratio is achieved by use of a plasma mirror, the proton emission from ultrathin foils (foils below 1 μm in thickness) is considerably enhanced [20]. This suggests that this is a highly suitable system for producing enhanced quasimonoenergetic proton beams. It is currently unclear what the best method for optimizing this process might be. In this paper we consider two of the approaches that have been proposed in the literature: microstructuring [14] and proton density reduction [21–23], in an intensity regime relevant to contemporary experiments. By means of three-dimensional (3D) kinetic simulations, we demonstrate that current experiments are unlikely to conform to the scheme originally proposed by Esirkepov *et al.* [11]. At intensities around 10^{19} W cm^{-2} high monochromaticity can only be achieved by drastically lowering the proton density of the microdot. Our findings suggest that the observations in recent experiments are actually due to the specific composition of the microdot, which is surprising given the high proton density of the latter ($\approx$50% H).

The first approach—microstructuring the rear surface of the foil—would ideally take the form of a single proton-bearing microdot on a substrate that contained no protons. The proposed mechanism is that a thin proton layer should be accelerated to a single energy; however, since the acceleration is nonuniform in the transverse direction along the rear surface this usually results in a broad energy spectrum. The use of the microdot target eliminates most of the lateral emission, which should narrow the energy spectrum. In a recent landmark experiment, Schwoerer *et al.* have demonstrated that this does result in a distinct peak in the energy spectrum [14]. The experiment was interpreted according to the scheme of Esirkepov *et al.* [11]; however, this comparison is questionable since the proton density in the microdot is very high. Additionally we should note that in [14], fewer than 0.01% of the protons were present in this quasimonoenergetic feature, whereas nearly all the protons should be accelerated according to [11]. The accompanying simulations in [14] were not reported on in sufficient detail to assess these issues. Moreover, this interpretation conflicts with 1D isothermal expansion theory, which says that even thin surface layers tend to expand to produce broad energy spectra [21,23,24]. This is because, at early times, the accelerating sheath field is screened out with a spatial scale corresponding to the cold Debye length, which is typically less than 1 nm. Even in situations where the protons are initially accelerated together, it is very likely that the space charge of the protons will quickly become significant, leading to a broadening of the energy spectrum.

The following physical arguments serve to demonstrate that if the proton layer strongly alters the local electric field structure by electrostatically screening out the sheath field, then this can lead to strong differential acceleration across the layer. Consider a hypothetical set-up with only a surface layer of thickness L and fast electrons. It is supposed that the bulk ions are immobile, the cold electrons are ignored, and the proton density is n_p. If the surface layer is thin, then one can take the fast electron density n_f inside it to be spatially uniform. In 1D, one can therefore directly integrate Gauss's law $\partial_x E_x = \rho/\varepsilon_0$ to find the variation in the electric field across the surface layer, $\Delta E_x = eL(n_p - n_f)/\varepsilon_0$. One can estimate the fast electron density to be about the relativistically corrected critical density ($\approx 10^{21}$ cm^{-3}), and the proton density must be that of the solid material ($\approx 10^{23}$ cm^{-3}). Even if the surface layer were 10 nm thick, one still finds $\Delta E_x \approx 10^{13}$ V m^{-1}. A ΔE_x of this magnitude would certainly cause a significant energy spread even up to intensities of $\approx 10^{20}$ W cm^{-2}. Since the accelerating electric field at early times is $E_x \approx \sqrt{n_f k_B T_f/\varepsilon_0}$, then taking $k_B T_f \approx 4$ MeV gives $E_{sheath} \approx 10^{13}$ V m^{-1}. Since $\Delta E_x \approx E_{sheath}$, one would expect a very broad energy spectrum. This leads to the conclusion that

the screening due to the proton space charge must eventually lead to a broad spectrum even if the layer is initially very thin.

In the case of very thin targets and high contrast, the fast electron density at the rear surface may be higher than the corrected critical density, but this needs to be verified by a fully self-consistent calculation. This may occur in the extreme cases such as the laser piston regime that occurs above 10^{23} W cm^{-2} as reported in [25]. In other 3D particle-in-cell (PIC) simulations at 10^{21} W cm^{-2} [11], it was found that monoenergetic beam production occurred in the case of a 1λ target where the initial substrate electron density was $9n_{crit}$ and the initial proton density was $0.25n_{crit}$, but the dependence on the proton density was not investigated.

Arguments similar to those above have led a number of researchers [21–23,26,27] to conclude that only targets containing protons in a relatively low concentration will produce a quasimonoenergetic peak in the proton spectrum. This is the proton density reduction approach. This may account for the observation of a quasimonoenergetic deuteron beam from a laser-irradiated water droplet [15], in which the deuterons were the minority species. This idea is based on considering the case of a relatively low density proton population among a lower charge-to-mass ratio ion species. In this situation the protons are not a significant electrostatic source term either in the bulk plasma, or up to a certain point in the electron sheath outside the bulk plasma. Since the bulk ions have a lower charge-to-mass ratio, and their dynamics determines the electric field structure, the protons undergo test-particle-like motion in an electric field that changes relatively slowly. This causes an accumulation in phase space, and thus a peak in the energy spectrum. This theory has been shown to work in different 1D kinetic (Vlasov) [23] and hybrid-kinetic [21,22] numerical models. However apart from being 1D, these models are essentially isothermal, which is not appropriate in the case of a very thin foil and a very short duration laser pulse. However, previous work has generally considered the case where the proton composition is less than 25%, with only the work in Ref. [23] suggesting that the heavy ions can induce a spectral peak at high proton density (above 50%).

We have carried out simulations in which we vary the proton density in a microdot, and a simulation with a foil that is 50% H and 50% D. We report on the results and we discuss to what extent these two theories explain the results.

The numerical code used here is the Pretty Efficient Parallel Coulomb Solver (PEPC) [28,29]. PEPC is a gridless particle code that directly solves for the Coulomb force between quasiparticles using multipole expansions to reduce the number of operations in the force summation to $O(N \log N)$. There are no Maxwell's equations as such, and the code is purely electrostatic. Laser absorption is included by means of a ponderomotive model, which includes both $\mathbf{v} \times \mathbf{B}$ heating and profile steepening at the critical surface. Comparisons with 2D electromagnetic PIC simulations show that the interaction physics is accurately described for "rigid," overdense targets such as those considered here [29].

The standard run (A) comprises a foil target of size $3.14 \times 1000 \times 1000 c^3 \omega_p^{-3}$ ($\approx 0.1 \times 30 \times 30$ μm^3), with an electron density of $16n_{crit}$. The laser is modeled with a normalized
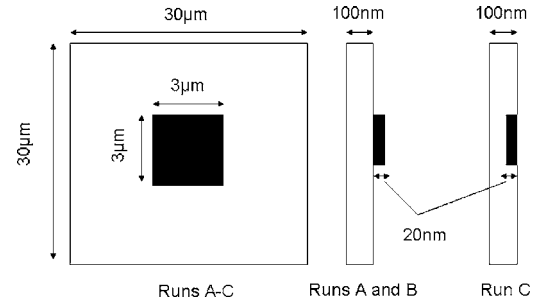

FIG. 1. Illustration of the target setup in runs A–C. Substrate foil is white and the microdot is black.

amplitude of $a_0 = 2.7$, a wavelength of 800 nm, a pulse duration of 35 fs (full width at half maximum), and a focal spot radius of $150c\omega_p^{-1}$ (≈ 4.8 μm). The plasma ions are deuterons ($Z=1, A=2$), the electron temperature is initially 300 eV, and the ions are initially cold. The protons are present as a microdot of transverse dimensions $100 \times 100c^2\omega_p^{-2}$, which is centered (axially and radially) and which extends $0.6c\omega_p^{-1}$ from the rear surface (≈ 20 nm). The microdot consists purely of protons at the same density as the foil. The spatial extent of the quasiparticles, ε, is set to $5c\omega_p^{-1}$. This means that the plasma is effectively collisionless. The simulations were run up to $1000\omega_p^{-1}$ (106 fs). In all runs the fast electron temperature was found to reach about 1–1.3 MeV.

Three other runs were also carried out. Run B is identical to run A, except that the microdot now consists of 50% H and 50% D. Run C is identical to run A, except that the protons are present as a doped region of the same dimensions but extending into the target. The proton density in the doped region is 4.7% that of the foil density. In run D the microdot was eliminated and the entire foil consisted of 50% H and 50% D. The reader may find Fig. 1, which illustrates the target setup in runs A–C, helpful.

We shall now describe the results of runs A–C. The proton energy spectra and proton phase space at $1000c\omega_p^{-1}$ are shown in Figs. 2 and 3, respectively. We observe a progressive narrowing of the energy spectrum as the proton density is decreased. The pure proton microdot (run A) produces the broadest spectrum (660 keV–6.6 MeV), with the 50% H
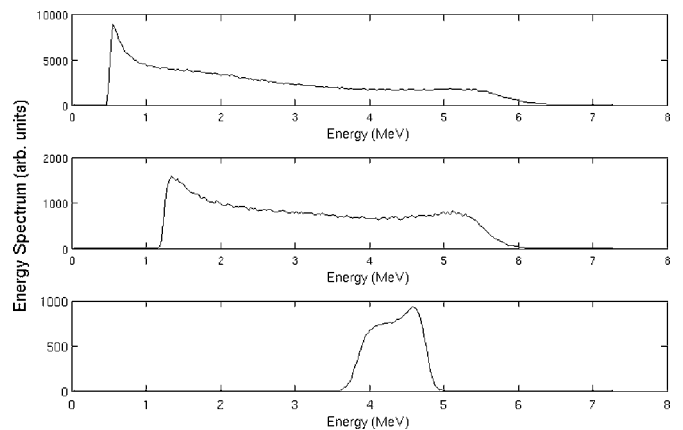

FIG. 2. Proton energy spectra of runs A (top), B (middle), and C (bottom), at $1000\omega_p^{-1}$.
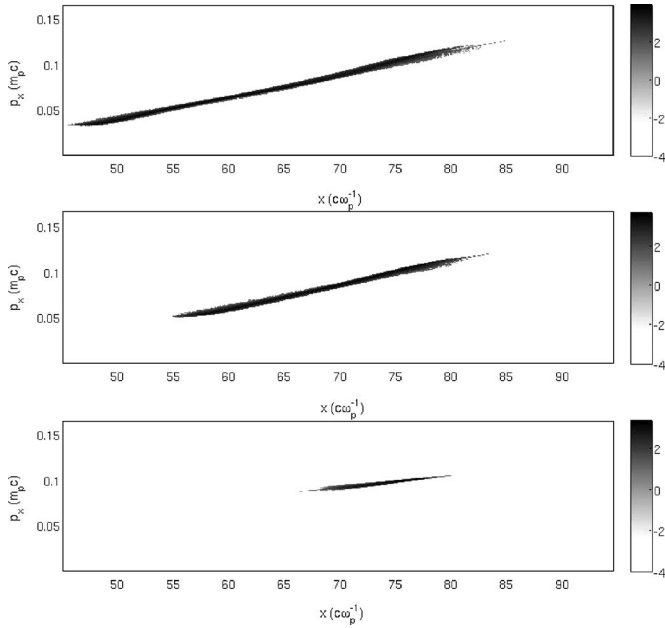
FIG. 3. Proton phase space of runs A (top), B (middle), and C (bottom), at $1000\omega_p^{-1}$.

microdot (run B) producing a slightly narrower spectrum (1.7–6.5 MeV). A quasimonoenergetic spectrum is seen in run C ($\Delta E = 900$ keV, with a peak energy of 4.6 MeV). The integrated proton velocity profile in runs A and B is a linear function, consistent with a plasma expansion process. The proton distribution function in run C consists of a localized bunch with a trailing tail. This is consistent with test-particle-like motion. We attribute this behavior to the reduction in the proton space charge, as we argued earlier.

The effect of the proton density on the electric field is clearly seen in Fig. 4 in which we show the electric fields and proton densities along $y=0$, $z=0$ at $500\omega_p^{-1}$ and $750\omega_p^{-1}$. In run A the electric field is altered strongly by the presence of the protons, i.e., two positive peaks in the field. In run C the protons have a negligible effect on the electric field, i.e., the field has a single positive peak.
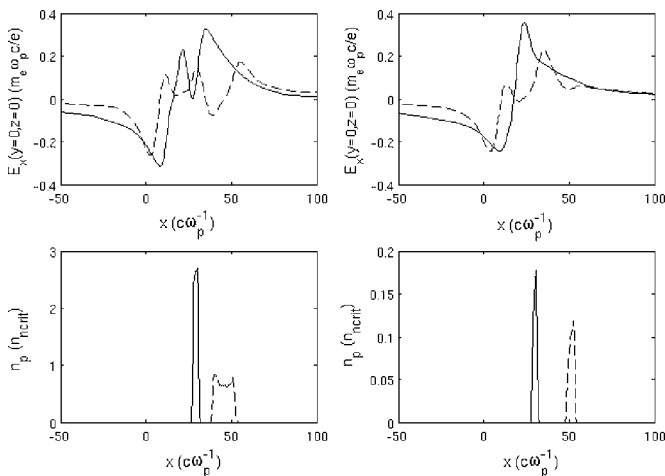

FIG. 4. Electric fields (top) and proton densities (bottom) in run A (left) and C (right) at $500\omega_p^{-1}$ (solid) and $750\omega_p^{-1}$ (dashed).
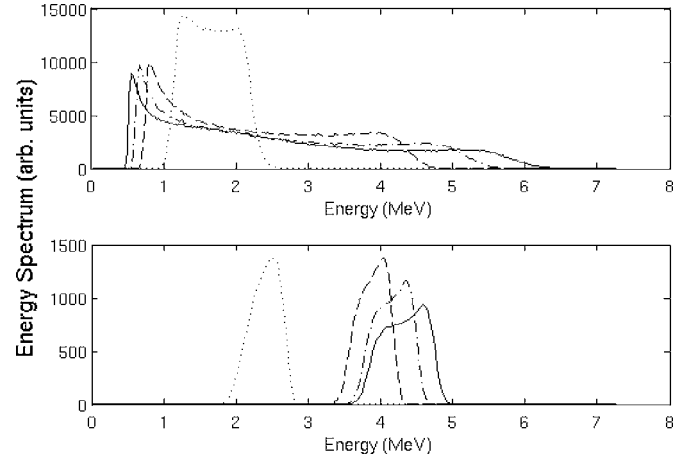

FIG. 5. Proton energy spectra in run A (top) and run C (bottom) at $1000\omega_p^{-1}$ (solid), $875\omega_p^{-1}$ (dash-dot), $750\omega_p^{-1}$ (dash), and $500\omega_p^{-1}$ (dot).

Although we have only carried out the simulation up to $1000c\omega_p^{-1}$, the proton spectra are approaching their asymptotic solutions. This is shown in Fig. 5 in which we show the spectra in runs A and C at four different times. Figure 5 also illustrates how the spectrum is strongly broadened throughout run A, and a quasimonoenergetic spectrum is maintained throughout run C.

It is interesting to compare all three simulations to a previous 1D isothermal model developed by one of the authors [23]. This simpler model predicted that, as the relative proton density is reduced, the maximum energy should decrease, and that a quasimonoenergetic spectrum could only be produced with a very low proton density. Importantly, we have now demonstrated this remains true without the constraint of either isothermal electrons or planar geometry.

The most interesting result however, is that run A does *not* produce a central peak in the spectrum. What this series of runs shows is that in order to recover the Esirkepov *et al.* scheme [11] (in this intensity regime) the proton density of the microdot must be drastically reduced. The proton density used by Schwoerer *et al.* [14] was far too high to yield a spectrum resembling that from run C. We suggest that more careful interpretation is required. The microdots in the Schwoerer experiment were not 100% H in composition. The polymethyl methacrylate (PMMA) monomer unit is $C_5H_8O_2$ so PMMA is only 53% H in composition. We therefore expect that run B should in fact be closer to describing the Schwoerer experiment, but this does not exhibit the small quasimonoenergetic feature seen in [14]. However, the microdot in the experiment was much thicker (0.5 μm), so we carried out a further run D to examine the acceleration from a thicker slab containing 50% H.

In run D the energy spectrum of the protons that are accelerated from a region of $150c\omega_p^{-1}$ around the center of the foil does contain a small quasimonoenergetic feature—Fig. 6. Qualitatively this spectrum compares quite favorably with the results from the microdot experiments (see also Fig. 3.25 in [30]). This quasimonoenergetic feature is associated with the deuteron front. In phase space it is a small accumulation of protons just ahead of a weak electrostatic shock at the ion
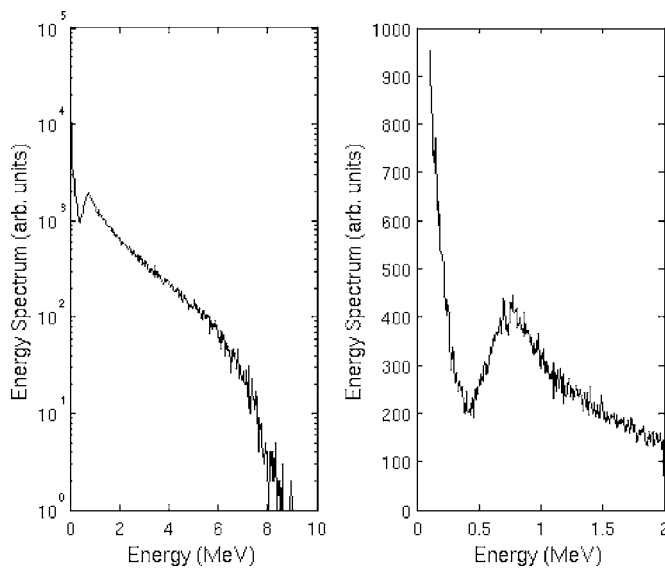
FIG. 6. Energy spectrum of protons within $150\omega_p^{-1}$ of the foil center in run D at $1240c\omega_p^{-1}$. Entire spectrum is on the left, and a closeup of the peak is shown on the right.

front, a feature that vanishes if the proton fraction is increased. The existence of such a feature at such a high proton fraction was not predicted by [11,21,22], but it was suggested by the previous 1D model in [23]. This spectral peak is absent in calculations with only one ion species. The microdot is still necessary to isolate this part of the spectrum, but it is not sufficient. Only when the proton density is reduced can this quasimonoenergetic feature be produced. If one considers the energy spectrum of a group of protons

that are emitted from a narrow region outside the central region then the spectrum is quasiexponential and without any peaks. We also note, by comparing runs B and D, that this mechanism works differently from the Esirkepov *et al.* scheme with respect to source thickness. If we thin the source region too much then the feature disappears (run B), and it is only present where the source region is sufficiently thick (run D). By contrast, Esirkepov *et al.* emphasized that the spectral width decreased with decreasing microdot thickness. This suggests that current experiments are being dominated by the proton fraction of the microdot, and not by the spatial localization of the protons.

In summary, we have carried out a set of simulations using a gridless kinetic particle code in order to compare the effect of limiting the proton source size against doped foils with reduced proton density. The results suggest that current experiments are not actually conforming to the Esirkepov *et al.* scheme, which only works with a very low proton density in the microdot. We have also demonstrated that the essential features of an important recent experiment appear to be determined by the proton fraction in the microdot, and that spatial localization of the protons alone is insufficient to explain the results, contrary to current understanding. If the 50% H microdot is made too thin, then the quasimonoenergetic feature disappears. This suggests that current results might best be improved by engineering the proton density in the microdot.

ACKNOWLEDGMENTS

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