Electron Self-Injection into an Evolving Plasma Bubble: The Way to a Dark Current Free GeV-Scale Laser Accelerator

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Electron Self-Injection into an Evolving Plasma Bubble: The Way to a Dark Current Free GeV-Scale Laser Accelerator

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Abstract. A time-varying electron density bubble created by the radiation pressure of a tightly focused petawatt laser pulse traps electrons of ambient rarefied plasma and accelerates them to a GeV energy over a few-cm distance. Expansion of the bubble caused by the shape variation of the self-guided pulse is the primary cause of electron self-injection in strongly rarefied plasmas ($n_0 \sim 10^{17}$ cm$^{-3}$). Stabilization and contraction of the bubble extinguishes the injection. After the bubble stabilization, longitudinal non-uniformity of the accelerating gradient results in a rapid phase space rotation that produces a quasi-monoenergetic bunch well before the de-phasing limit. Combination of reduced and fully self-consistent (first-principle) 3-D PIC simulations complemented with the Hamiltonian diagnostics of electron phase space shows that the bubble dynamics and the self-injection process are governed primarily by the driver evolution; collective transverse fields of the trapped electron bunch reduce the accelerating gradient, slow down phase space rotation, and result in a formation of monoenergetic electron beam with higher energy than test-particle modeling predicts.

Keywords: Laser wakefield acceleration, self-focusing, self-guiding, blowout regime, electron trapping, PIC simulations

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INTRODUCTION

Since the first demonstrations a half-decade ago [1], laser wakefield accelerators (LWFA) have made an impressive progress towards producing GeV-scale electron beams from cm-long plasmas [2]. Both electron acceleration and laser self-guiding [3] are associated in these experiments with a unique plasma structure — electron density bubble [4, 5] — created by the ponderomotive force of a laser pulse focused to the relativistic intensity, $I > 10^{19}$ W/cm$^2$. The bubble forms when all plasma electrons facing the pulse are expelled by the radiation pressure (while fully stripped ions remain immobile). Fields due to this charge separation attract bulk electrons to the axis, and their trajectories overshoot. The resulting closed cavity of electron density surrounded by a dense shell (sheet) of relativistic electrons propagates with a near-luminous speed over a positive ion background; the associated Lorentz factor is $\gamma_b \approx \omega_0 / \omega_{pe} \gg 1$, where $\omega_0$ is the laser frequency, and $\omega_{pe} = \left(4\pi e^2 n_0/m_e\right)^{1/2}$ is the electron plasma frequency (here, $m_e$ is the electron rest mass, $n_0$ is the background electron density, and $e$ is electron charge). Some of the sheath electrons can get into the bubble near its rear end (where the accelerating electric field has the maximum), synchronize with it (i.e. obtain longitudinal momentum $p_L \approx m_e c \gamma_b$), and then travel inside the cavity over a long distance and continuously gain energy. However, both simulations [2, 3] and the experiment [6] agree that the bubble formation is not a sufficient condition of self-injection and formation of collimated electron beam. The problem of self-injection becomes particularly tough for the planned LWFA experiments with short-pulse petawatt (PW) lasers [7], in which case the sheath electrons are unlikely to pick up with the ultra-relativistic bubble ($\gamma_b \sim 100$). One way to enforce injection has been recognized long ago, and this is to cause the bubble expansion by either introducing a density down-ramp in the direction of propagation [8] or taking advantage of the de-focusing of strongly over-focused driving pulse [9]. Revision of the latter approach [10, 11] has shown that the laser diffraction followed by self-guiding is the most attractive scenario for the formation of a monoenergetic electron beam. As the over-focused laser diffracts, the bubble expands, and electrons are injected continuously. As the diffraction ceases, and self-guiding sets in, the bubble stabilizes, and self-injection terminates. In this case, the secondary injection in the same bucket (dark current) is suppressed, and the low-energy tails [2] do not show up in the electron energy spectra. The bubble remains large during the self-guided stage, hence the electrons injected during its expansion travel deeply inside the bucket and get continuously accelerated. Importantly, electrons injected immediately before the bucket stabilization are situated in the region of the
FIGURE 1. (Color online). Snapshot of laser wake field from the cylindrically symmetric WAKE simulation. Arrows in panels (a) and (c) point in the direction of pulse propagation. Panel (a): cavity of electron density in the wake of the laser pulse [yellow/light gray broken line (black in other panels) — intensity iso-contour at exp(-2) of the maximum]; the cavity is surrounded by an electron sheath of sub-micron thickness. Sample macro-particle trajectories in panel (b) are color coded according to their dynamical behavior (see discussion in the text). Panels (c)–(e) show the wake potential, accelerating and focusing gradients, and the trajectory of the innermost sheath electron (broken yellow/light gray curve).

highest accelerating gradient. They rapidly equalize in energy with earlier injected particles, and monoenergetic bunch forms well before the nonlinear de-phasing [3] occurs. In this report we examine this scenario numerically using both reduced and fully explicit electromagnetic three-dimensional particle-in-cell (EM 3-D PIC) codes.

First, we examine the motion of relativistic electron fluid surrounding the bubble. We emphasize the quasistatic nature of this motion and evaluate the minimal growth rate of the bubble sufficient to enforce self-injection. Next, we verify this estimate in test-particle modeling of electron self-injection in the non-stationary quasistatic bubble driven by a quasi-paraxial laser pulse, associate the details of self-injection process with the features of laser evolution, and support these considerations with a non-stationary Hamiltonian diagnostics. The simulation is done using the code WAKE [4]. Finally, we validate the test-particle modeling using fully explicit EM 3-D PIC simulations using the code CALDER-Circ [12]. We find that in strongly under-dense plasmas \[n_0 \sim 10^{-4}n_e \sim 10^{17} \text{ cm}^{-3}\], where \[n_e = m_e\omega_0^2/(4\pi e^2)\] is the critical density the test-particle modeling has high predictive capability and is able to correctly identify the physical processes responsible for the initiation and termination of self-injection.

QUASI-STATIC ELECTRON FLOW SURROUNDING THE BUBBLE.

In the remainder of this report we concentrate on a regime typical of the planned Texas Petawatt experiments [14]. We take 15 mm length plasma of density \(n_0 = 10^{17} \text{ cm}^{-3}\); there are 0.3 mm length linear density downramps at the entrance and exit. The laser pulse with a central wavelength \(\lambda_0 = 1.054 \mu\text{m}\), 200 J energy, and full width at half-maximum in intensity \(t_L = 150 \text{ fs}\) is focused at the foot of the front ramp (\(z = 0\)) into the spot of radius \(r_0 = 27.35 \mu\text{m}\) \((k_p r_0 \approx 1.63\), where \(k_p = \omega_0/c\)). The pulse is overcritical for the relativistic self-focusing, \(P \approx 8P_{cr}\), where \(P_{cr} = 16.2n_e/c_0\) GW. Its peak intensity \(I_{\text{peak}} = 1.153 \times 10^{19} \text{ W/cm}^2\) corresponds to the normalized vector potential \(a_{\text{peak}} = 9.62\). Upon entering the plasma, the strongly mismatched pulse \((k_p r_0 \ll 2\sqrt{a_0})\) is expected to diffract as in vacuum until nonlinearities balance diffraction. The simulation uses the grid \(d\xi = 0.05c/\omega_{pe} = 0.8a_0\), \(dr = 1.5d\xi\) with 30 particles per radial cell, and takes 20 hours on a single-core 2.13 GHz Intel processor with 1 GB RAM.

Figure 1 shows the plasma bubble after 0.5 mm of propagation. Electron density, sample trajectories of macro-particles \(r_c(z - ct)\), wake field potential, and time-averaged (over \(\omega_0^{-1}\)) Lorentz forces are extracted from the cylindrically symmetric PIC simulation via code WAKE. WAKE macro-particles obey the quasistatic approximation (QSA) and thus cannot be trapped. However, analysis of their trajectories allows to define a group of particles – trapping candidates, and specify the scenario of bubble evolution favorable for injection. Examination of trajectories [Fig. 1(b)] and phase space of the macro-particles \(p_c(z - ct)\) (not shown) indicates that each electron can be put into one of three clearly defined groups [these are color coded in Fig 1(b)]. The majority of plasma electrons, either expelled by the radiation pressure (blue/gray), or bulk electrons attracted to the axis by the charge separation force (green/light gray), are passing. They fall behind the bubble within a time interval roughly equal to the bubble duration.

Electrons that form the sheath (red/dark gray) are different. Unlike the other two groups, they travel with the bubble
FIGURE 2. (Color online). Panel (a): peak laser intensity (red/gray) and bubble length (black) as a function of propagation distance. Hamiltonian characterization of test electron phase space (Fig. 3) is applied at the position labeled “a”. Panel (b): test electron energy at the end of the plasma ($z = 1.5$ cm) as a function of initial position of test electron. All accelerated electrons were collected by the expanding bucket during the interval of laser diffraction (from $z = 0.3$ to 3.4 mm). As the laser becomes self-guided, bubble expansion stops, and injection never resumes.

over extended period of time: calculation shows that the slippage time of a sheath electron through the structure, $T_{\text{slip}} = \int_{\xi_{\text{tail}}}^{\xi_{\text{initial}}} d\xi / (c - v_z)$, may be 2 to 5 times longer than the bubble duration (here $\xi = z - ct$, and $\xi_{\text{tail}}$ is the point of trajectory crossing). And, according to Figs. 1(d) and (e), they are exposed to the strongest wake fields over this time interval (note that the peak values of both accelerating and focusing gradients exceed the cold wave breaking limit, $E_{\text{WB}} = m_e \omega_{pe} c / |e| \approx 0.3$ GV/cm). As a consequence, electrons approaching the point of trajectory crossing are pre-accelerated to multi-MeV energy [for Fig. 1(b), $\gamma_{\text{max}} \approx 20$]. They are apparently the best trapping candidates, and lifting the QSA restrictions could facilitate their injection and acceleration [13]. Their longitudinal momentum, however, is yet too low for the synchronization with the bubble ($\gamma_{\text{max}} \sim \gamma_b / 5$); therefore, were the bucket “frozen” (i.e. depending on variables $r$ and $z - ct$ only) these electrons would slip along the rim of the bucket and remain passing.

In order to get injected, the non-quasistatic sheath electron has to slip into the cavity and stay there over sufficient time to gain enough energy to synchronize with the bucket. Or, conversely, the bubble has to expand, in which case some of the heavy sheath electrons lag behind the moving bubble boundary and stay inside the bubble. Apparently, the bubble must be expanding rapidly enough to change its size by an appreciable fraction during the slippage time $T_{\text{slip}}$. To facilitate separation of most energetic electrons from the sheath, minimal increment of the bubble size over the slippage time $\Delta L_b(T_{\text{slip}})$ has to exceed the thickness of the sheath $\Delta_{\text{sh}}$ near the bottom of the bubble:

$$\Delta L_b(T_{\text{slip}}) \geq \Delta_{\text{sh}}; \quad (1)$$

Our previous work [7, 10, 11] shows that the condition (1) holds every time when robust self-injection occurs in the simulations. We shall demonstrate it once more in the next section.

FIGURE 3. (Color online). Hamiltonian analysis of trapped electron beam after the bubble stabilization [position labeled “a” in Fig. 2(a)]. (a) Electron density bubble. Top — quasistatic electron density; bottom — radial positions of test electrons; dashed curve — laser intensity iso-contour at $\exp(-2)$ of the peak. (b) Blow-up of the region highlighted with red box in panel (a). Test electrons are color coded according to the value of MF Hamiltonian [black: $H_{\text{MF}} < 0$ (trapped); green/light gray: $0 < H_{\text{MF}} < 1$ (injected); red/dark gray: $H_{\text{MF}} > 1$ (passing)]. (c) Longitudinal momentum of electrons versus positions of their injection. Earlier injected electrons ($0.3 \text{mm} < z < 2.7 \text{mm}$) are trapped ($H_{\text{MF}} < 0$); electrons injected before the bubble stabilization ($2.7 \text{mm} < z < 3.4 \text{mm}$) do not satisfy the sufficient condition for trapping ($0 < H_{\text{MF}} < 1$). (d) MF Hamiltonian versus energy gain: both trapped and injected electrons are accelerated to the same energy.
ELECTRON SELF-INJECTION INTO EXPANDING ELECTRON DENSITY BUBBLE: TEST-PARTICLE MODELING AND HAMILTONIAN DIAGNOSTICS.

Quasi-static nature of the accelerating structure makes it possible to examine and understand the physics of electron self-injection (initiation, termination, phase space rotation) using conceptually simple and computationally efficient toolbox: a fully relativistic 3-D particle tracking module built into the cylindrically symmetric time-averaged quasistatic PIC code WAKE. The test-particle module is non-averaged in time, fully dynamic, and does not assume cylindrical symmetry; in particular, it takes into account the interaction of test electrons with non-averaged linearly polarized laser field. To emulate the laser pulse interaction with non-quasistatic background electrons (and thus to model self-injection into non-stationary quasistatic wake fields), a group of quiescent test electrons (with $γ = 1$) is placed before the laser pulse at each time step. Specific features of electron self-injection associated with the bubble and driver evolution are thus disentangled from the effects brought about by the collective fields of the trapped electron bunch (nonlinear beam loading) [15]. This simulation toolbox allows to fully characterize the details of self-injection process [7, 11] and relate them to the structure dynamics using non-stationary Hamiltonian formalism [16].

Figure 2 correlates self-injection of test electrons with the structure evolution. Panel (a) shows that the pulse diffracts as in vacuum upon entering the plasma, and the bubble size $L_b$ (a distance between the first maximum and first minimum of the potential $Φ$ on axis) starts growing as soon as the laser reaches the density plateau. Panel (b) indicates that only these electrons are accelerated and reach the end of the plasma ($z = 1.5$ cm) which were collected by the bubble during the period of its expansion. According to Fig. 2(a), the bubble expands by 0.3% of its size as it propagates over the length $L_b$. Using the estimate of the slippage time from the previous section, $T_{slip} \sim 4L_b/c$, we find $ΔL_b(T_{slip}) \approx 1.2 \times 10^{-2}L_b \approx 0.9$ μm, which is close to the grid size-limited thickness of the sheath near the point of trajectory crossing, $Δ_{sh} \approx 0.8$ μm. Hence, the results of test particle modeling agree with the qualitative condition (1).

As the laser becomes self-guided, the bucket size stabilizes, and self-injection ceases. Although the self-guided laser remains intense enough to maintain electron evacuation in the first bucket, self-injection never resumes.

WAKE code uses Hamiltonian variables, which makes the Hamiltonian analysis of the test particle tracking straightforward. Using the definitions $γ_e = \sqrt{1 + \frac{p^2 + a^2}{m^2} / 2}$, $p \equiv \frac{p}{(m_c)}$ (normalized momentum), $Φ \equiv |e|(Φ - A_z)/(m_c)$ (normalized wake potential), $a \equiv |e|a/(m_c^2)$ (normalized slowly varying amplitude of the laser vector potential), we introduce the normalized time-averaged moving-frame (MF) Hamiltonian $H_{MF}(r, z - ct) = γ_e + Φ + p_z$. For the quasistatic WAKE macro-particles $H_{MF} = 1$. A non-quasistatic test electron moves in explicitly time-dependent potentials; hence, its $H_{MF}$ changes in the course of propagation according to $dH/dt = ∂H/∂r$. For a test electron moving away from the bubble after the interaction, $H = γ_e + Φ - p_z = √{1 + \frac{p^2}{m^2} - p_z > 0}$. Hence, the electron will be confined inside the bucket at all times if the MF Hamiltonian becomes negative in the course of interaction.

Once the bubble stabilizes, the MF Hamiltonian of test electrons is conserved. All test electrons can now be divided into 3 groups: (1) $H < 0$ — trapped electrons (sufficient condition satisfied); (2) $0 < H < 1$ — injected (accelerated) electrons (sufficient condition not satisfied); (3) $H > 1$ — passing electrons. All the three groups are represented in Fig. 3 which shows the plasma bubble soon after its stabilization (position “a” in the left panel of Fig. 2). It can be seen

![FIGURE 4](image-url)

FIGURE 4. (Color online) Phase space rotation and formation of monoenergetic electron beam. Panel (a) — longitudinal phase space of test electrons at (A) $z_A = 0.75$ mm; (B) $z_B = 3.45$ mm; (C) $z_C = 5.1$ mm; (D) $z_D = 14.7$ mm. (b) Axial line-outs of the accelerating gradient at the same positions. At the position (A) injection begins. Positions (B) and (C) correspond to the stabilized bucket. Injection stops, and phase space rotation begins at $z = z_B$; at $z = z_C$ electrons near the tail of the bubble (exposed to the highest accelerating gradient) pick up in energy with the earlier injected ones. Further phase space rotation increase the energy spread [position (D)].
immediately that the condition $H_{MF} < 0$ need not be fulfilled to achieve the effective acceleration. In the presented example, electrons with $0 < H_{MF} < 0.9$ are accelerated as effectively as those which are trapped ($H_{MF} < 0$); and their numbers are roughly the same. The conclusion is that reduction of the MF Hamiltonian, $H_{MF} < 1$, is the necessary condition for acceleration. In the considered regime with ultra-relativistic bubble, $\gamma_b \geq 100$, it appears to be almost sufficient. Finding the small decrement $\Delta H = H_{MF} - 1$ sufficient for acceleration is the subject of future work.

As soon as the bubble stabilizes [position (B) in Fig. 4], injected electrons become exposed to the longitudinally non-uniform stationary accelerating gradient. Tail of the bunch ($0 < H_{MF} < 0.9$) is exposed to a higher gradient than earlier injected (trapped) electrons. Figure 4 shows that within the interval 1.65 mm after the bubble stabilization [distance between (B) and (C)], tail and head equalize in energy, and monoenergetic bunch is produced (relative energy spread $\approx 2\%$). This happens well before reaching the nonlinear de-phasing limit, $L_{d} = (2/3)(n_e/n_0)L_b \approx 50$ cm [3].

**INJECTION INTO EXPANDING BUBBLE: FULLY EXPLICIT 3-D PIC SIMULATION**

Collective fields of the relativistic electron bunch, neglected in the test-particle treatment, are known to change the shape of the sheath and thus reduce accelerating gradient, arguably bearing responsibility for the termination of self-injection [15]. In this section, we verify the test-particle results by running a fully explicit EM 3-D PIC simulation with the identical set of laser and plasma conditions. We use a newly developed massively parallel code CALDER-Circ [12], which has a computational efficiency of a 2-D PIC code due to the decomposition of fields into a set of poloidal modes. The simulation uses two lowest-order radiation modes. The time step $dt = 0.124/\omega_0$ and the grid $dz = 0.125c/\omega_0 = 0.02\lambda_0$, $dr = 20dz$ are chosen so as to suppress the numerical dispersion in the direction of propagation; 15 macro-particles per toroidal cell are used. Simulation runs in a moving window and takes 32500 CPU hours (130 hours on 250 cores) on “Titan” cluster at CEA, which is 1600 times longer than the WAKE run. Figure 5 shows that despite a much coarser grid and underlying approximations, WAKE-based simulation toolbox correctly captures all relevant physics of plasma wake evolution and dynamics of electron self-injection. In addition, CALDER-Circ modeling correctly recovers the evolution of electron phase space after termination of injection. Despite a great difference in the algorithms, both codes recover the same correlation between the laser and bubble evolution. Self-injection can be thus characterized as trapping the relativistic projectile by the time-varying 3-D potential well. From the position “a” to “b” in panel (vii) the laser pulse diffracts as in vacuum, while the bubble expands. Pre-accelerated sheath electrons with high inertia ($\gamma_e \gg 1$) lag behind the boundary of expanding bubble, and stay inside the bucket (injected charge is $\sim 1.3$ nC in the CALDER-Circ run). Stabilization of the bubble in the

![FIGURE 5](https://example.com/figure5.png)

**FIGURE 5.** (Color online). (i)–(iii): Electron density at the positions (a)–(c) in panel (vii). Top half of the panels: bubble with self-injected electrons from the CALDER-Circ simulation. Bottom half: quasistatic bubble from the WAKE simulation (injected test electrons not shown). (iv)–(vi): longitudinal phase space for the same positions. Color map shows macro-particle density in the phase space from CALDER-Circ simulations. Yellow/light gray dots — WAKE test particles. Panel (vii): same as left panel of Fig. 2. Panel (viii): energy spectrum of CALDER-Circ macro-particles and WAKE test particles from the panel (vi).
vicinity of position “b” extinguishes injection and thus limits the injected charge. Remarkably, in both WAKE and CALDER-Circ simulations injection starts and terminates at exactly the same positions along the propagation axis; the laser wake thus remains quasistatic along the entire interaction region despite of considerable injected charge, and its evolution is governed primarily by the driver evolution. The shape and size of the bucket are strikingly the same in both runs. Beam loading in the CALDER-Circ run results in a slight sheath distortion at the rear end of the bucket [as seen in panels (ii) and (iii)], which plays no role in the initiation or termination of self-injection. As the beam loading is unable to prevent the bubble stabilization and contraction, the tail of the bunch gets truncated; electrons remaining in the bucket experience phase space rotation. Beam loading, however, reduces the longitudinal inhomogeneity of accelerating gradient and thus slows down the phase space rotation. The monoenergetic electron beam thus forms much later in the CALDER-Circ simulation than in the WAKE simulation (around $z \approx 14.7$ mm instead of $z \approx 5.1$ mm), and its central energy is 2.3 times higher (460 MeV instead of 200 MeV). The root-mean-square energy spread, however, remains the same, $\sim 2\%$. Comparison of the electron energy spectra at the exit of the plasma [panel (viii)] shows that the test-particle spectrum in the absence of beam loading develops a high-energy tail; curiously enough, it still reveals a monoenergetic feature at the same energy as in the CALDER-Circ run ($E = 460$ MeV). This feature corresponds to the earlier injected electrons which form the front tip of the bunch unaffected by beam loading.

CONCLUSION

Electron self-injection into the expanding bubble of electron density underlies the performance of multi-cm-long GeV-class plasma accelerators driven by a self-guided PW laser [7]. Natural pulse evolution (nonlinear focusing, defocusing and self-steepening) is in most cases sufficient to initiate and terminate the injection. The bubble dynamics and the self-injection process are governed primarily by the driver evolution. Although collective transverse fields of trapped electron bunch reduce the accelerating gradient and slow down phase space rotation after the bubble stabilization and termination of injection, quasi-monoenergetic electron bunch forms well before de-phasing. Evolution of the accelerating gradient and thus slows down the phase space rotation. The monoenergetic electron beam thus forms much later in the CALDER-Circ simulation than in the WAKE simulation (around $z \approx 14.7$ mm instead of $z \approx 5.1$ mm), and its central energy is 2.3 times higher (460 MeV instead of 200 MeV). The root-mean-square energy spread, however, remains the same, $\sim 2\%$. Comparison of the electron energy spectra at the exit of the plasma [panel (viii)] shows that the test-particle spectrum in the absence of beam loading develops a high-energy tail; curiously enough, it still reveals a monoenergetic feature at the same energy as in the CALDER-Circ run ($E = 460$ MeV). This feature corresponds to the earlier injected electrons which form the front tip of the bunch unaffected by beam loading.

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