PARTICLE-IN-CELL MODELING OF DIELECTRIC WAKEFIELD ACCELERATOR*

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Abstract

We explore the potential of Dielectric Wakefield Accelerator (DWA) to achieve compact high gradient acceleration of high brightness beams required by an Xray Free Electron Laser (FEL). Particle-In-Cell (PIC) simulations of a LANL DWA experimental design utilizing a double triangle beam current profile indicate accelerating field >100 MV/m and large transformer ratio are accessible while the longitudinal wakefield phase is insensitive to beam parameters and radial offset for fixed longitudinal profile. End-to-end simulation is developed, which allows us to validate and optimize future DWA experimental design.

INTRODUCTION

The pre-conceptual design for Matter-Radiation Interactions in Extremes (MaRIE) future signature facility at LANL calls for a 12 GeV electron linear accelerator for hard X-ray FEL production. MaRIE demands a high quality electron beam with the electron bunch charges of 0.1 to 1 nC, normalized RMS emittances of 0.1 to 1 mm, and RMS energy spreads of less than 0.1%. A major deficiency of the conventional accelerator technology is the accelerating gradient that is limited to a few tens of MV/m, which put a severe restraint on the cost and future upgrade of such facility.

The wakefield which causes the dominant energy spread in beams in conventional linacs can be used in carefully designed electromagnetic structures, specifically, dielectric loaded waveguides in this study, to generate extraordinary gradients and potentially small energy spreads for electron beam acceleration. In this paper we present simulation study to assess the characteristics of DWA and its potential applications in advance of experimental validation.

THEORY ON WAKEFIELD IN DWA

Figure 1 shows the schematic of the dielectric-lined metallic waveguide. Here we confine our study to a waveguide with cylindrical symmetric geometry. The theory of wakefield generation in a cylindrical dielectric waveguide is generally formulated in frequency domain and dated back at least to 1951 in Ref. [1], where Bessel's equation for the fields is solved with boundary matching conditions at the dielectric-vacuum interface. In general, the dielectric-lined waveguide supports infinite number of discrete Hybrid EM modes. The supported EM modes have low frequency cut-off determined by the geometric

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Figure 1: A schematic of the DWA consisting of a dielectric-lined metallic waveguide and an electron beam as the excitation source.

parameters of the waveguide and the dielectric constant ε of the liner materials.

However, for axial symmetric excitation (azimuthal mode number m=0), the TE and the TM modes are decoupled. For co-linear particle acceleration, the TM_{0n} modes are most useful for particle acceleration via the strong longitudinal electric field. While TE modes are detrimental to acceleration but can be used for beam deflection.

In Ref. [1], the dispersion of the TE, the TM and the HEM eigen modes are derived. Similar efforts are found in Ref. [2-4] for resonant modes driven by a moving particle. Here we adopt the notation used in Ref. [3] and summarize the key results relevant to our interests below:

(1) The conditional equation (dispersion relation) for modes with phase velocity $v_{ph} = \beta = v/c$,

$$C(s) = \frac{m^2 sk^2}{a^2} \beta^2 \left(\frac{\varepsilon - 1}{1 - \beta^2}\right)^2 - s^3 \left(\frac{kS_m(sa)}{S_m(sa)} + \frac{sI_m(ka)}{I_m(ka)}\right) \left(\frac{sI_m(ka)}{I_m(ka)} + \frac{\varepsilon kR_m(sa)}{R_m(sa)}\right) = 0$$
(1)

where $k^2 = \omega^2 (1 - \beta^2)/v^2$, $s^2 = \omega^2 (\epsilon \beta^2 - 1)/v^2$, $k_0 = \omega/c$, and R_m , R'_m , S_m , S'_m are combinations of *m*th–order Bessel functions of the first and second kinds as defined in Eq. (35-38) in Ref. [3].

(2) The TM_{mn} longitudinal electric field for a single particle (Green's function),

$$E_{z,mn}(r,\theta,z-vt) = -8e\cos(m\theta)\cos\left(\frac{\omega}{v}(z-vt)\right)$$

$$\times I_m(kr)I_m(kr_0) \times \frac{K_m(ka)}{I_m(ka)} \frac{T(s)}{sdC(s)/ds}\Big|_{s=s}$$
(2)

where

$$T(s) = -\frac{m^2 k^4 \beta^2}{a^2} \left(\frac{\varepsilon - 1}{1 - \beta^2}\right)^2 - s^2 k^2 \left(\frac{k S'_m(sa)}{S_m(sa)} + \frac{s I'_m(ka)}{I_m(ka)}\right)$$
$$\times \left(\frac{s K'_m(ka)}{K_m(ka)} + \frac{\varepsilon k R'_m(sa)}{R_m(sa)}\right)$$

and s_n is the solution of Eq. (1).

To obtain the wakefield generated by a beam, one can convolve (sum) the single particle field from Eq. (2) with the beam profile. For smooth beams, this can be done

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with sufficient accuracy using the first few modes excited. However, this procedure will involve more modes if the beam profile has a large Fourier content. A more efficient method is the expansion of the fields into the orthonormal modes of the dielectric waveguide [5]. In addition, evanescence modes that co-move with the beam have to be taken into account for Gauss's law to be satisfied [6].

DWA PROTOTYPE EXPERIEMENT

We attempt to combine the concepts of the dielectric wakefield acceleration and the Emittance Exchanger (EEX) [7] in a unique way to experimentally demonstrate a high-brightness DWA with an acceleration gradient exceeding 100 MV/m and with less than 0.1% induced energy spread in the accelerated beam. The designed DWA parameters are listed in Table 1. ELEGANT simulation is used to track the beam through the beam line elements to the entrance of the DWA. More detail about the beam optics to produce the double triangle drive beam current profile and a witness beam can be found in Ref. [7]. Theoretical analysis [8] indicates that a double triangle drive beam can excite a wakefield with large (>2) transformer ratio.

Table	1: D	WA	Parameters
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Parameter	Value	
Inner/Outer radius b/a	0.57 mm / 0.662 mm	
Dielectric constant ε	3.75	
TM mode cutoff freq.	298 GHz	
Drive/Witness beam charge	5 nC / 250 pC	
Drive/Witness beam length	2.35 ps / 100 fs	

(0) (1)

PIC SIMULATION OF DWA

Figure 2: Comparison of theoretical prediction and MERLIN simulation result for the longitudinal wakefield driven by a double triangle beam.

We use PIC codes MERLIN [9] and LSP [10] to model the DWA in 2D cylindrical (r, z) and 3D (r, θ, z) geometries, respectively. We first conduct benchmark with analytic DWA theory presented in Ref. [3] using the same dielectric waveguide parameters defined in Table 1, but with a longer 4 ps, 5 nC, 100 MeV double-triangle

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beam of a temporal profile described by f(t) = t for $0 \le t$ ≤ 0.85 ps and f(t) = t - 0.52 (*ps*) for 0.85 ps $\le t \le 4$ ps.

The MERLIN simulation uses stationary box of size 0.662 mm × 30 mm. The simulation box is divided into 133×6000 cells. The dielectric material is placed at 0.57 mm < r < 0.662 mm. The cell size is 0.00498 mm × 0.005 mm and the time step is 11.7 fs. The electron beam is injected from the boundary at z=0 mm. 1600 macroparticles per cell is used for the beam. Perfect Electric Conductor is used at the boundaries at z=0 mm and r = 0.662 mm. Transmitting boundary for particles and fields is used for the boundary at z=30 mm.

Benchmark Result

The longitudinal wakefield in the simulation and the analytical result based on the formalism described in previous section are compared in Fig. 2. The simulation lineout is taken at radius R=0.37 mm when the beam has propagated 2.464 cm into the DWA. Good agreement between the simulation and theoretical result is seen for the wakefield generated in the beam (the decelerating field) and behind (periodic accelerating and decelerating fields). Lineout on the axis shows similar agreement but is noisier. The deceleration field within the drive beam is nearly flat, which is a consequence of the double-triangle drive beam current profile and important for a high transformer ratio (in this particular example, $E_{dec} \approx 17.5$ MV/m and $E_{\rm acc} \approx 117$ MV/m, leading to a transformer ratio of about 6.7). The difference at t > 35 ps is due to the transient behavior of the wake excitation near the DWA entrance



Figure 3: Comparison of the wakefield generated by onaxis beam (MERLIN) and off-axis beam (LSP, shifted by 20 μ m at θ =0) at t=41 ps. The simulation lineouts are taken at R=0.04 cm and θ =1.5, 4.5.

When the transverse shape of drive beam is varied among a radial flat-top profile with radius of 0.2 mm (result shown in Fig. 2) and a Gaussian profile with spot size of 0.165 mm and 0.0825 mm respectively (not shown), the longitudinal dependence of the longitudinal wakefield shows little variation in overall shape but different noise levels (noisier for narrower beam). The former observation is consistent with Eq. (2) where the longitudinal and radial dependences are completely separate. On the other hand, higher longitudinal resolution simulation indicates that the noise is a numerical artifact, which mostly results from under-resolving the sharp edge of the double triangle beam. The wakefield of an off-axis beam in LSP simulation is compared to the MERLIN simulation and the theory in Fig. 3. The result shows that its longitudinal dependence is largely unaffected by the shift as the theory predicts.

End-to-End Simulation of DWA



Figure 4: The on-axis beam current density (black) from the ELEGANT and the calculated cut-off radius (red) for the symmetrized Gaussian beam distribution.

Although our benchmark shows reasonable agreement between the DWA analytical theory and simulation, experiment conditions are often non-ideal, requiring more realistic simulation to validate the experimental observations and to optimize the design. It is important that this can be done in an end-to-end type simulation where beam particles are tracked through various beamline elements and modeled self-consistently in the DWA. For this purpose, we started developing a link between the beam tracking code ELEGANT and the electromagnetic PIC codes. We have built such a prototype code for linking with the 2D cylindrical code MERLIN. The particles are taken from the ELEGANT simulation, resampled (described below) and injected into MERLIN simulation, while the transverse beam fields are first calculated in a quasi-static solver similar to Ref. [11] and subsequently imported into the MERLIN simulation as initial conditions. For relativistic beams, the beam fields are predominantly quasi-static fields and the longitudinal fields can be ignored, therefore a quasi-static solver would be sufficient (an advantage of this approach is the removal of the image charge at the DWA entrance in the simulation). Because of the cylindrical nature of the MERLIN code, we need to apply an extra step to slice and symmetrize the beam particle population (not necessary in 3D simulation). We assume the beam has a cylindrically symmetric Gaussian shape at the entrance of the DWA and calculate a cut-off radius according to the following formula for each slice,

$$Q(z) = 2\pi \int_{0}^{R_{cut}} \frac{J_{b0}(z)}{e} e^{-r^{2}/\sigma_{r}^{2}} r dr$$
(3)

where Q(z) and $J_{b0}(z)$ are the total charge and on axis longitudinal current density of the each beam slice from the ELEGANT data.

Figure 4 shows the calculated cut-off radius using this approach. Figure 5 shows the charge density of the beam

injected into the MERLIN simulation and the longitudinal wakefield generated in the DWA.



Figure 5: (Top) The on-axis beam charge density in an end-to-end simulation of DWA using MERLIN and input from ELEGANT and parameters in Table 1. Both drive and witness beams propagate to the left. (Bottom) The longitudinal wakefield generated (x_1 in cm and E_1 in MV/m). An accelerating field >100 MV/m together with a transformer ratio >3 are observed. The field noises are mostly due to the under-resolved sharp edge of the beam.

SUMMARY

We have carried out 2D and 3D PIC simulations of the DWA concept for potential application in high gradient compact accelerator. Simulations show good agreement with the analytic DWA theory for the accelerating field, the transformer ratio and the longitudinal dependence of the accelerating field with respect to the transverse beam shape and offset. End-to-end simulation shows that the LANL proof-of-principle DWA design can achieve an accelerating field >100MV/m and a transformer ratio >3.

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