Projected next-generation linac-based light sources such as PERL or the TESLA free-electron laser (FEL) generally assume, as essential components of their injector complexes, long-pulse photocathode rf electron guns. These guns, due to the nature in which they are operated, may be more susceptible to ion bombardment damage of their cathodes than conventional rf guns. This paper explores this possibility and presents a basis for future study of the subject.

Introduction

Current designs for next-generation linac-based light sources, whether they are proposed as dedicated machines (e.g., PERL) or as parts of other high-energy accelerators (e.g., TESLA FEL), tend to have certain common design features. The proposed linacs are usually either entirely or mostly superconducting in order to allow long bunch trains and high duty-factor operation. Average beam currents tend to be high, on the order of 0.1 – 1 A. The rf frequency is typically L-band (1.3 GHz) as a compromise between cavity construction concerns and projected performance.

Naturally, the injectors for these proposed machines are typically also L-band (although there are exceptions, e.g., a proposed subharmonic gun based on the Boeing high-duty-factor gun for PERL). High quantum efficiency (QE) cathodes are also taken to be essential parts of the injector design, given the laser power requirements for copper, magnesium, or other low-QE materials. Typical high-QE cathodes, however, have generally been found to be much more sensitive to environmental conditions such as residual gases in the gun than lower-QE materials.

In general, no cavity can be rendered completely free of residual gases. Therefore, the passage of the electron beam through the photocathode rf gun can result in ionization of the residual atmosphere. This is true for any photoinjector. However, for the photoinjectors envisioned for future light sources, there are several important differences from those commonly used today. First, these guns are to be operated at high accelerating gradients on timescales ranging from milliseconds to true continuous wave (CW) operation, as opposed to a few microseconds for more conventional guns. Second, rather than generating a single electron bunch, these guns are anticipated to produce long-duration bunch trains by placing electron bunches in a large fraction of the available rf “buckets.” In the case of PERL, for instance, it is anticipated that every bucket may in fact be filled. The result is the continuous creation of ions and the continuing presence of strong fields, which may cause the ions to migrate in a preferred direction inside the gun. In DC guns, in general any (positive) ion created will backstream to the cathode. In rf guns the situation is more complex due to the rapidly time-varying rf fields. In this paper the propagation of ions in a typical photoinjected rf gun design is explored and some initial results presented. It concludes with directions for future work if so warranted.
Simulation Methodology and Parameters

Initial Assumptions

Several assumptions are used throughout this initial study.

First, the source atoms or molecules are assumed to be uniformly distributed within the volume of the gun. They are assumed to be converted to ions only from impact by the electron beam. Ionization from dark current, secondary emission electrons, the incoming photocathode drive laser pulse, or the rf field itself, is neglected.

Second, no multiple ionization events are assumed to take place. Similarly, after the initial “generation” (i.e., start of the simulation) no ions are assumed to become deionized through electron capture.

Third, ion-ion interactions are not included. The validity of this assumption will be verified later.

Finally, the ions are assumed not to be strongly affected by either the magnetic field of the focusing solenoid typically located at or close to the output port of many photoinjeter designs or by the magnetic field of the electron beam. In the simulations done to date, the maximum ion kinetic energy (for hydrogen) corresponds to a velocity of about 0.5% of the speed of light, so this is a reasonable assumption.

Simulation Model

The basic design of the gun used in the simulation is a fairly traditional SLAC/BNL/UCLA-type 1.5-cell cavity with a resonant frequency of 1.3 GHz. The detailed gun geometry was provided by Manoel Conde of the Argonne Wakefield Accelerator (AWA) group at Argonne National Laboratory. The poisson/superfish codes were used to generate the required fields from the model geometry, shown in Figure 1.

The simulation code PARMELA was used to perform the actual particle tracking. The simulations were generally run with timesteps of one degree of L-band phase (approximately 2.14 ps); selected runs were performed at shorter timesteps to verify that the one-degree increment provides reasonable accuracy. Ion particle locations were recorded at regular intervals during the tracking.

In order to determine the appropriate starting phase of the rf field in the gun, a reference electron bunch was propagated from the cathode, with a launch phase of 35 degrees following the zero-crossing, and average gun gradient of 34.5 MV/m; this provides for an exit electron beam energy of 7.3 MeV and represents a typical operational gradient for the AWA gun used as the simulation model. The reference particle flight path is used to determine the phase of the rf field when the electron beam reaches a given longitudinal position within the gun. For a given longitudinal coordinate, ion starting locations are specified via an external file. Assuming the initial gas species have uniform density in the gun, the ion macroparticle radial coordinates are chosen so as to place the particles in the center of equal-area rings. Thus, assuming an equal probability of ion creation, each ion macroparticle represents an equal number of actual ions.
Once the simulation is started, the ion macroparticles are tracked until all have either impacted a wall or the simulation time expires. No multiple ionizations are assumed to take place while the ions are in motion. In the case where the gun may be used for single-bunch operation, i.e., during tuneup, this is a reasonable assumption. When operating bunch trains, however, there is a definite possibility of multiple ionization events for species other than hydrogen, and electron capture and deionization is also always a possibility. These effects are beyond the current capabilities of PARMELA, but could be included in a purpose-written code.

If the simulation assumes single-bunch operation then there is no field from an on-axis electron beam to influence the ion motion. In multibunch operation, however, there is a pulsed on-axis electron beam, the fields of which can influence the ion motion. The effects of these fields are approximated in the simulation by including the field from an on-axis charged cylinder, with charge uniformly distributed along the length of the gun and with a charge density such that the total on-axis charge contains 1 nC along the distance traveled by an electron bunch in one rf period. Since the ions move slowly compared to the electron beam, this distribution in effect simulates the field averaging the ions would see as many bunches are generated and transit the gun. This method does not include the effects of the electron beam magnetic field, however these effects are taken to be small. Also, the electron beam transverse size will change as the beam moves through the gun; this is also not taken into consideration. The generated electrostatic potential is shown in Figure 2.

Finally, the simulation ignores the starting motion of the ions, e.g., they are assumed to start at rest instead of a velocity taken from some distribution based on kT. The validity of this assumption was verified by imposing a velocity distribution on the input beam and noting that this had little to no discernable impact on the ion flight tracks. Since the fields in the gun are symmetric, ions are placed out only along one axis (typically +x or +y).

Simulation Results – H⁺ Ions

We begin by considering what happens to hydrogen ions starting at a specific longitudinal coordinate and at varying radii and ignore for the moment whether a particular ion macroparticle would be within the electron beam radius at that longitudinal position. The use of hydrogen eliminates the multiple ionization assumption. Hydrogen may be derived from any number of molecular species such as methane, water, ethanol, etc., so assuming its presence in a gun is probably reasonable. Ion starting positions are chosen with a longitudinal spacing of 0.5 cm, from 0.5 cm to 17.0 cm from the cathode. Radial starting positions and starting phases are selected as described above.

Some sample ion tracks for hydrogen atoms are shown in Figure 3. Note that depending on the starting location (and thus time), the ions can have very different flight paths through the gun. Some starting locations have ions directed towards the cathode in a broad spray; some result in ions being trapped between the cathode and full cell; and some result in well-collimated streams of ions being either ejected from the gun or directed towards the cathode. Figure 4 combines data from plots such as those shown in Figure 3, from all of the launch positions, into an impact energy plot. The (z,r) location in the plot shows the assumed ion starting location, and the color of the point represents the impact energy at the cathode plane. For these plots, a single-shot electron beam is assumed, e.g., no effects of an on-axis electron beam are included. Figure 5 is an impact energy plot for hydrogen including
the effects of an on-axis electric charge on ion propagation, as described above, assuming a bunch charge of 1 nC and every bucket filled. There are differences due to the on-axis fields, but the overall distributions are very similar and the peak impact energies are also nearly the same.

The H\(^+\) ion tracks and impact energies show very strong dependence upon the time and location of ionization. The H\(^+\) ions that impact the cathode plane were found to gain kinetic energies of up to almost 13 kV, or about 4·10\(^5\) the average thermal energy (for room-temperature cavities). The potential wells formed by the electron beam, in contrast, are on the order of 300 V at most, for 1-nC charge per bucket and every bucket filled. Therefore, it is not surprising that the presence of the on-axis charge distribution does not generate a significant shift in the impact-energy plots in terms of final impact energy from a given starting location and phase. There is a noticeable difference on the ion trajectories, however, which also shows up as a strong influence on the ion impact distribution over the cathode plane.

This also illustrates why H\(^+\) ions starting at rest and with some thermal velocity distribution show very little difference in their trajectories; the ions quickly accelerate up to many times the thermal velocity. Tests were done assuming a distribution of starting energies based on \(kT\), but no significant impact upon the particle tracks were found.

Finally, the impact energy distribution on the cathode is determined. The impact energy plots in Figures 4 and 5 only illustrate which particle starting locations result in ions impacting the cathode plane; it does not show where the ions deposit their energy on the cathode. Because the particle starting locations are tracked, we may histogram the impact energy based on all ions started either within a given radius (e.g., to model the ion generation of an electron beam with uniform transverse distribution) or within a given cylindrical shell (e.g., to help model the effects of an electron beam with a nonuniform transverse distribution).

Figure 6(a) shows the impact energy histogram on the cathode plane for a 1-cm radius about the axis of the gun, assuming that no on-axis charge is present; Figure 6(b) assumes an on-axis charge equivalent to 1 nC per bunch, every bucket filled. The histogram bin widths are scaled to represent equal area rings on the cathode plane. In both figures the red curves include only ions generated within 0.5 cm of the gun’s axis, while the blue curves include all ion starting locations. The presence of a high beam current is seen to be beneficial in that it provides, in effect, a strongly overfocusing lens that acts to diffuse the hydrogen ion current over a larger area of the cathode.

The scaling factor to translate between the arbitrary units shown and the actual energy (or power) deposited on the cathode depends on the partial pressure of hydrogen within the gun (or molecular species from which it may be liberated), the electron bunch charge, the number of electron bunches generated (or, for power calculations, the beam repetition rate), and the probability of ionization.

In any event, the ion flight paths and impact energy histograms indicate that the model L-band photoinjector is fairly good at funneling H\(^+\) ions towards the cathode and that the ions can impact with significant energy. This alone indicates possible problems for long-pulse
operation with high-QE cathodes, especially if a relatively low average current is generated. Somewhat surprisingly, these results indicate that the use of higher beam currents may in some circumstances actually help to preserve cathode longevity by more uniformly distributing the ion impacts on the cathode plane. This would have to be balanced, however, against the greater rate of ion production from the continuous presence of the electron beam.

**Simulation Results - H$_2$O$^+$ Ions**

Simulations were also performed using ions with mass equivalent to singly-ionized water molecules. These simulations therefore include the assumptions that multiple ionization does not take place and that the water molecule is not disassociated due to repeated interactions with the electron beam, in addition to the other assumptions used for the hydrogen simulations. The ion starting positions and phases were selected in the same fashion as described above for H$^+$ ions.

Impact energy plots for water ions are shown in Figure 7, which assumes no on-axis electron beam charge distribution, and Figure 8, which assumes the nominal 1-nC charge per bunch, every bunch filled. There are very significant differences between the two impact energy plots, and the impact energy is in general much reduced from the case of H$^+$ ions presented above.

The reasons for these differences may be explained as follows. Consider both an H$^+$ ion and a water ion (approximately 18 times as massive) in the field of the gun. The field accelerates the particles and they begin to move; however because of their mass the acceleration is very low, at least compared to an electron. One complete rf period later, the ion will have been induced to drift somewhat, and depending on the field uniformity at the starting location after one rf period, the ion may be returned to rest or may have acquired some drift velocity. The amount of drift velocity increase will depend on the local field uniformity. Therefore, one would expect the ions to gain most of their momentum in the regions where the rf field intensity has a large gradient with respect to position, e.g., near the nosecones; and, examining the H$^+$ flight paths shown in Figure 3, this is seen to be the case. All other things being equal, the more massive the ion, the smaller the distance it will move in a single rf period; therefore, it will acquire a smaller velocity kick. Thus, one would expect that hydrogen ions would pick up energy faster, and obtain a higher final energy, than heavier species. This is confirmed with the results of the H$_2$O$^+$ ion tracking.

For this reason, the relative effect of on-axis charge's fields should be greater for heavier ions than for lighter ions; the field from the on-axis electron beam is effectively a DC field (on the timescales of the ion motion) and therefore does not rely on a positional change and local field gradient to impart an acceleration. This is in fact the case observed for H$_2$O$^+$, where there is clearly a strong change in the particle impact energy distribution and potential source points from the presence of the on-axis charge. One would not expect, however, the thermal distribution to play a greater role as the mass of the ion species increases because the starting velocity of the ions would decrease as the mass of the species is increased. This is in fact the case; as was the case for the H$^+$ ions, there is little obvious difference between the ion tracks of H$_2$O$^+$ ions with and without an imposed thermal velocity distribution, based on a temperature of 300K.
Finally, we use the results of the hydrogen simulations to determine, for the case of 1-nC charge per bunch and every bucket filled, the amount of hydrogen ions impacting on the cathode per second.

The ionization rate per unit volume is given by

\[
\frac{dn}{dt} = n_b n_g \sigma_i v,
\]

where \( n_b \) is the density of the electron beam, \( n_g \) is the density of the gas species, \( \sigma_i \) is the ionization cross-section and is about \( 2 \times 10^{-23} \) m\(^2\) at the average electron beam energies in the gun, and \( v \) is the beam velocity. Expressed in terms of the total number of hydrogen ions created per rf period, this may be rewritten as

\[
\frac{dN}{dt} = \frac{Q_b P \sigma_i c}{e k_B T D},
\]

where \( N \) is the total number of ions generated, \( Q_b \) is the bunch charge, \( P \) is the partial gas pressure, \( \sigma_i \sim 2 \times 10^{-23} \) m\(^2\), \( c \) is the speed of light, \( e \) is the electron charge, \( k_B \) is Boltzmann’s constant, \( T \) is the temperature in Kelvin, and \( D \) is the duty factor expressed in terms of the fraction of possible rf buckets filled. The electron beam density \( n_b \) is taken as an average and is calculated by dividing the bunch charge by the volume swept out by the bunch in a single rf period. Note that the physical dimensions of the electron beam (e.g., radius) do not appear when expressed in this fashion. We can also calculate the number of ions generated per beam pulse as

\[
N_p = \frac{dN}{dt} \frac{\tau_{rf}}{D} = \frac{Q_b P \sigma_i c}{e k_B T f_{rf}},
\]

where \( \tau_{rf} \) is the rf period, and \( f_{rf} = 1/ \tau_{rf} \) is the resonant frequency of the cavity. Note that if the bunch charge, gas pressure, or ionization cross-section are low enough, this can result in an ion production rate of less than one per rf period. Note also that the rate of ion production scales inversely with temperature, meaning that for the same pressure, superconducting rf guns should have much higher rates of ion creation than normal-conducting rf guns.

Next, from the \( H^+ \) simulation with the on-axis charge distribution, we find that, of the ions generated within 0.5 cm of the bore, approximately 1/3 of the generated ions will impact on the cathode. Using a 1-nC bunch charge, a duty factor of 1 (i.e., every bunch filled), and a partial pressure of hydrogen of \( 10^{-13} \) Torr, we obtain a hydrogen ion current to the cathode of 64 fA assuming CW operation. The mean impact kinetic energy of these ions is approximately 7 kV, for a power delivery to the cathode of 0.5 nW. This is the total beam
current delivered to the entire cathode surface, however we know from Figure 6(b) that most of this current is going to be impacting close to the center of the cathode plate.

This is a low rate of energy delivery to the cathode and, based on the results for water ions, should be even lower for more massive species. The delivered current scales directly with the partial pressure of the species inside the gun. It also scales with the average electron beam current; however, as the beam current can have an influence on the ion trajectories, the exact scaling is more complex. This simple calculation also does not take into account the steep rise in ionization cross-section for electron beam energies in the $10^1 - 10^5$ eV range, which can be as high as $10^{-20}$ m$^2$. This potentially represents a much larger source of ions in the vicinity of the cathode, which would immediately backstream towards the cathode. It should also be noted that for the case of water ions, when an on-axis charge distribution was assumed, the ions with the greatest impact energy were generated in the vicinity of the cathode (see Figure 8).

Based on the calculated ion current, the initial approximation of ignoring ion-ion and ion-beam interaction is probably reasonable, given the other approximations made. The simulations do, however, show evidence of ion trapping within the gun close to the nosecones between the cathode and full cells. With sufficient rf pulse duration and average beam current, one could conceive of an ion charge buildup large enough to have an impact on the electron beam and ion flow. For the beam and gas parameters listed above, and assuming that 10% of the ions generated are trapped, it would take approximately 86 minutes to generate and trap 100 pC of hydrogen ions, assuming no deionization takes place, the generation and capture process is not adversely affected by the local buildup of space charge, and the assumptions regarding the CW electron beam approximation are valid.

Conclusions and Future Directions

Long-pulse rf guns may experience deposition of energy upon their cathodes from lighter ionized species such as hydrogen. This is more true for high average beam current guns, where the ions will be continually generated and pumped towards the cathode. The actual ion current of a given species towards the cathode will depend on the partial pressure in the gun, the average beam current in the gun, and the ionization cross-section, but, given these parameters, the above results can provide at least an estimate of the potential for damage. The ions resulting from the interaction between the relativistic electron beam and the residual gas do not result in a large current flow to the cathode; however, the much larger ionization cross-section near the cathode surface (where the beam is under 0.1 MeV in kinetic energy, for instance) may prove to be cause for concern, especially if the gun fields are good at transporting ions towards the cathode surface. This would require further study.

The methods used in this work are relatively straightforward and may be extended in any of several possible directions. For example, a more reasonable model of the electron beam propagation in the gun could be used to incorporate the time-varying electric and magnetic fields from the beam upon the ion flow. The possibility of multiple ionization events could also be incorporated, although this would require greater modifications to existing codes. Also, the electron beam energy gain profile could be used to better determine the ionization cross-section at any point in the gun. At this point, however, it does not appear as though ion beam currents in long-pulse photocathode rf guns pose significant risks to cathode
longevity as long as the residual species partial pressures, particularly of lighter species, are well controlled.

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Figure 1: Basic geometry of the model gun used in these simulations. The rf field lines are shown. The gun is cylindrically symmetric about the z-axis.
Figure 2: Equipotentials in the gun generated via an on-axis uniform charge distribution.
Figure 3: Hydrogen ion trajectories for four different longitudinal starting coordinates, and no electron beam field. Trajectories are color-coded to ion energy (red = minimum, blue=maximum for each individual plot). $z_{\text{launch}}$ and $\phi_{\text{launch}}$ are, respectively, the starting longitudinal coordinate and starting phase for the ions (e.g., $\phi_{\text{launch}}$ is the phase at which the centroid of a reference electron beam bunch reaches $z_{\text{launch}}$).
Figure 4. Impact energy at the cathode plane as a function of starting location. Red indicates the highest impact energy, dark blue indicates lowest. No on-axis charge is assumed.
Figure 5. Impact energy at the cathode plane as a function of starting location. Red indicates the highest impact energy, dark blue indicates no impact. On-axis electron charge is equivalent to 1 nC per bunch, every bunch filled.
Figure 6. Impact energy histogram for hydrogen ions generated within 0.5 cm of the gun axis (red), and for all ion starting locations (blue). Figure 6(a) assumes no on-axis beam charge; Figure 6(b) assumes 1-nC bunch charge, every bunch filled.
Figure 7. Impact energy plot for H$_2$O$^+$ ions, assuming no on-axis charge distribution. Note that the vertical scale is reduced one order of magnitude from the H$^+$ plots.
Figure 8. Impact energy plot for H$_2$O$^+$, assuming a 1-nC bunch charge and every bucket filled. Note that the vertical scale differs from both the H$^+$ and that in Figure 7.


5 Manoel Conde, Argonne Wakefield Accelerator, private communication