

SIMULATIONS OF ION MIGRATION IN THE LCLS RF GUN AND INJECTOR*

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Abstract

The motivation for this work was the observed surface contamination of the first LCLS RF gun copper cathode. We will present the results of simulations in regards to ion migration in the LCLS gun. Ions of residual gases will be created by interaction of molecular gas species with the UV drive laser beam and by the electron beam itself. The larger part of those ionized molecules remain in the vicinity of creation, are transported towards beam line walls or away from the cathode. However a small fraction gains enough kinetic energy, focused by RF and magnetic fields and propagates to the cathode, producing an undesirable increase of the cathode's surface work function. Although this fraction is small, during long term operation, this effect may become a significant factor limiting the source performance.

INTRODUCTION

The trajectories of common residual ionized gases have been simulated within the 1.6 cells of the LCLS RF gun and its immediate vicinity. A similar study has been carried out by Lewellen [1] and it has been shown that the potential of ion back bombardment in an RF gun is a real possibility. Furthermore, the surface analysis of the first LCLS cathode provides evidence for complex hydrocarbon contamination [2]. This study is conducted with the specific LCLS design parameters (RF and magnetic fields, and RF pulse structure). Typical partial pressures of residual gases in the LCLS gun during operation are high 10^{-10} Torr in the gun itself and low to mid 10^{-9} Torr immediately downstream. The assumption is that the UV laser drive pulse and the electron beam ionize residual gases that propagate towards the cathode surface. Simulations of the ion trajectory in the presence of RF fields and the magnetic field of the emittance compensating solenoid were performed using the General Particle Tracer software [3]. The ions studied were H^+ , CO^+ , CO_2^+ , CO_2^{2+} , CH_4^+ and CH_2^{2+} . The path of the ionized gas species and their kinetic energy were evaluated to study their contribution to possible cathode surface contamination. Finally, it was attempted to evaluate the time that is necessary to deposit ionized residual gas species on the cathodes surface.

SIMULATIONS

To set up the simulations, a cylindrical volume with the laser drive beam diameter was filled with particles of single or double charge and appropriate mass to represent the ionized residual gas species. One set of simulations was performed with particles originating only from within the gun, a second set with particles extending to 0.5 m

beyond the gun into the downstream beam line (Gun To Linac beamline (GTL)). Their motion was tracked over a time interval of 1.2 μs , which is the gun RF pulse duration of the LCLS injector. The particle distribution at the end of this time period served as input distribution for the next 1.2 μs RF cycle. 5000 particles were tracked for the duration of 100 1.2 μs long RF pulses. Post processing of the particle distributions at the end of each RF cycle was performed to generate the trajectories of species. The analysis discriminates between particles that are accelerated away from the cathode and particles that reach the cathode plane. For the latter case, the kinetic energy distribution was also determined. Particles that would be lost on beam line component walls were not excluded for the reason of simplicity.

SIMULATION RESULTS

Typical trajectory patterns are given in fig. 1 and 2 for double ionized carbon dioxide ions (CO_2^{2+}). Fig. 1 depicts the trajectory of the entire particle assembly and fig. 2 those reaching the cathode plane. Tables 1 and 2 summarize the fractions of the initial particle set reaching the cathode and their kinetic energy for ions generated inside the gun's 1.6 cell cavity and for an initial distribution that extends to 0.5 m downstream of the cathode plane. Only a small number will reach the cathode with low kinetic energy and becomes lower if

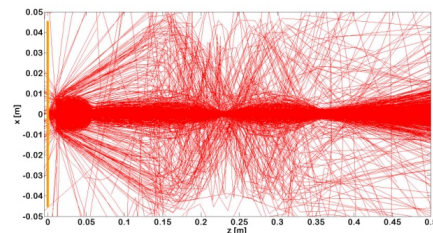


Figure 1: CO_2^{2+} particle trajectory for entire assembly.

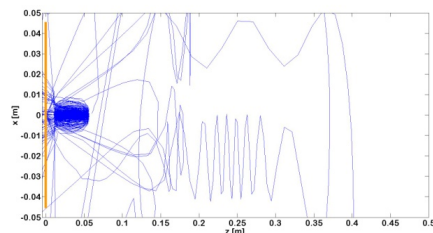


Figure 2: CO_2^{2+} particle trajectory for particles reaching the cathode.

particles further away from the cathode plane are considered. Fig. 3 plots the kinetic energy as a function of

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the specie's charge to mass ratio. The highest kinetic energy is observed for H⁺ ions (largest charge/mass ratio) and decreases as the charge to mass ratio becomes lower. The kinetic energy distribution for H⁺ ions propagating to the cathode plane is plotted in figure 4.

Table 1: Summary of simulation results

Species	Origin	Fraction reaching Cathode	E _{kin(max)} [eV]
H ⁺	Gun only	0.046	1.1E+04
CO ₂ ⁺	Gun only	0.012	1.5E+02
CO ₂ ²⁺	Gun only	0.043	2.2E+02
CO ⁺	Gun only	0.014	7.0E+01
CH ₄ ⁺	Gun only	0.035	1.7E+02
CH ₄ ²⁺	Gun only	0.026	1.3E+02
H ⁺	Gun & GTL	0.007	3.5E+01
CO ₂ ⁺	Gun & GTL	0.002	1.0E+01
CO ₂ ²⁺	Gun & GTL	0.003	1.7E+01
CO ⁺	Gun & GTL	0.002	9.0E+00
CH ₄ ⁺	Gun & GTL	0.003	1.4E+01
CH ₄ ²⁺	Gun & GTL	0.003	1.4E+01

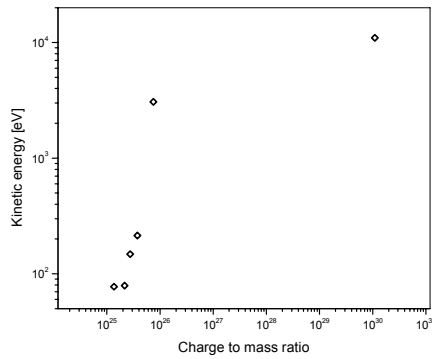


Figure 3: Maximum Kinetic energy at the cathode plane as a function of charge to mass ratio.

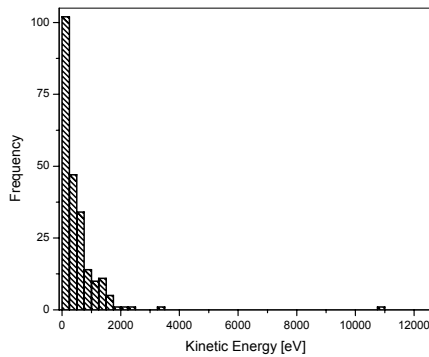


Figure 4: Kinetic energy distribution for H⁺ ions at the cathode surface plane.

IONIZATION RATE

The rate of ionization of typical residual gases can be estimated using the ideal gas law and the cross sections for photo ionization and electron-impact ionization. For example, the number of molecules at 300 deg K and a partial pressure of 10⁻⁹ Torr can be calculated according to:

$$n_{molecules} = \frac{P}{k_B T} = 3.2 \times 10^7 \text{ molecules / cm}^3$$

The number of ions produced is determined by the respective cross section and interaction length. An example of the electron impact cross section vs. electron energy is given in fig. 5 (C₆H₆). The interaction length for electrons is the distance over which the cross section is large (see fig 5). In this case:

$$L_{interaction} = \frac{T(eV) = 1KeV}{50MV / m} \approx 20microns$$

$$\begin{aligned} N_{ions,e} &= N_e \sigma_{C_6H_6} n_{molecules} L_{interaction} \\ &= 6.25 \times 10^9 e^- \times 10^{-15} cm^2 \times 3.2 \\ &\quad \times 10^7 \text{ molecules / cm}^3 \times 20microns \end{aligned}$$

$$N_{ions,e} \approx 0.4 \text{ ions / nC}$$

The calculation for photoionization of the residual gas by the UV laser gives an even lower ion rate.

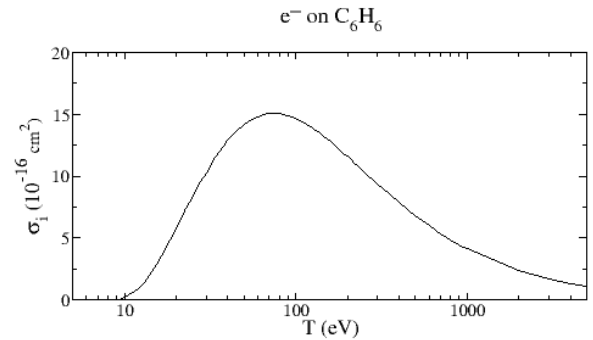


Figure 5: Ionization rate for C₆H₆ [4].

Another surface contamination possibility is the ionization of molecules which are first physisorbed onto the surface of the cathode and subsequently are chemisorbed upon ionization by laser photons or electrons. An estimate of the dynamics of this mechanism is give below. The molecular flux on the cathode surface is [5]:

$$\Gamma = n \sqrt{\frac{kT}{2\pi m}}$$

Where n is molecular volume density, m is the mass of the C_6H_6 molecule. At 10^{-9} Torr:

$$\Gamma = 3.2 \times 10^{13} \text{ molecules/m}^3 \sqrt{\frac{1.38 \times 10^{-23} \text{ J/deg K} \times 300 \text{ deg K}}{2\pi \times 78 \times 1.67 \times 10^{-27} \text{ kg}}}$$

$$= 2.3 \times 10^{11} \text{ molecules/(cm}^2\text{s)}$$

The monolayer formation time is then (assuming the area occupied by each deposited molecule is $d_0^2 \sim (10 \text{ angstroms})^2$)[5]

$$t_{ml} = \frac{1}{\Gamma d_0^2} = \frac{1}{2.3 \times 10^{11} \times (1 \times 10^{-7})^2} \approx 430 \text{ seconds}$$

with a monolayer having approximately 10^{14} molecules/cm².

The ion yield at the surface with 100 μJ (for $\sim 1\text{nC}$) of laser at 4.8 eV is then:

$$n_{ion} = 2 \times 1.3 \times 10^{14} \gamma' s / 100 \mu\text{J} \times 10^{-26} \text{ cm}^2 \times 10^{14} \text{ molecules/cm}^2$$

$$n_{ion} = 260 \text{ ions} / 100 \mu\text{J}$$

Since the laser runs at 30 Hz and beam size diameter is 1.2 mm, the time to decompose 10% of the monolayer is:

$$\frac{10^{14} / \text{cm}^2 \times \pi \times (0.06 \text{ cm})^2 (0.1 \text{ coverage})}{260 \text{ ions} \times 30 \text{ Hz}} \approx 1.5 \times 10^7 \text{ s} = 174 \text{ days}$$

For LCLS operating at tenths to hundreds of nC/s the ion contamination due to electron-impact and photoionization of the residual gas appears to be too small to explain the QE hole. Thus it appears the layer of adsorbed neutral molecules accumulated over several monolayer formation times is being photo-ionized into its constituents which then strongly bind to the surface and increase the work function.

SUMMARY

Ionization of residual gas species in the LCLS gun vacuum can occur by photo-ionization and electron impact within the volume of the gun itself or adjacent areas and also at the surface of the cathode itself. A small fraction of species originating from the volume of gun and adjacent areas can propagate to the surface of the cathode. However, the decomposition of the monolayer of absorbed residual gas species that is absorbed on the cathode surface is a more likely source of hydro-carbon contaminants which increases the cathode's work function and reducing the quantum efficiency.

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