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LINAC simulation with dataset generator

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Abstract
A dataset generator was developed for Axcelis' higher energy ion implanters, specifically for the Purion XEmax. At its core it uses a LINAC simulation to verify that the generated LINAC parameters achieve the desired particle energies with acceptable beam transmission. The LINAC simulation is an in-house written particle dynamics code that uses the equation of motion for alternating electric fields in the RF range.

Introduction

Axcelis' high energy ion implanters employ radio frequency linear accelerator technology (RF LINAC). The LINAC itself requires many parameters that need to be determined appropriately for optimal acceleration of the ion beam with good transmission and beam current. In particular, the Purion XEmax is equipped with two LINACS [1], each of which employs a multitude of resonators and electrostatic quadrupoles. Each resonator has an RF amplitude as well as a phase setting, effectively doubling the number of parameters. In addition, Boost™ Technology between the two LINACS can increase the charge state significantly to achieve higher energies with the same RF amplitudes [1]. A set of the large number of LINAC and booster parameters is called a dataset. A complete recipe set includes the LINAC dataset as well as all the other ion implanter settings such as those for the ion source, AMU magnet, final energy magnet, and corrector magnet, as well as dose to name the most relevant ones. For Axcelis' high energy legacy ion implanters look-up tables were meticulously generated in the past covering various species from minimum to maximum energy in fixed energy increments. If energies in between these steps is required some manual modifications of the dataset and further tuning is required. To generate look-up tables for the Purion XEmax would be a daunting task considering the even larger parameter space that is made available by the two LINACS and Boost™ Technology. Currently, once a customer requires ion implantation of a specific species such as Boron, Phosphorus, and Arsenic at different energies and charge states on the Purion XEmax Axcelis' equipment engineers will stepwise tune the LINAC to generate a dataset**,** typically at the factory, which is stored in the recipe and then transferred to the customer. In addition, Axcelis is continuously improving and upgrading their ion implanter fleet, making manual dataset generation a never-ending task. For all these reasons an automated dataset generator is highly desirable. In the next sections we will describe how this can be accomplished utilizing a LINAC simulation program that finds appropriate voltages, phases, and quad settings (dataset generator). This combination of software tools can create new datasets automatically and in a short period of time. Not only is such a dataset generator fast and convenient, but it can also be applied to any arbitrary ion species and energy making it very flexible. In addition, it can be constrained to generate equal RF amplitudes on each resonator, so that the maximum electric stress for each resonators is kept to a minimum improving reliability.

Purion XEmax and two gap acceleration

As described elsewhere [1] the Purion XEmax is an ultra-high energy implanter specifically design for the CMOS Image Sensor industry, which can achieve maximum energies up to 15 MeV for Arsenic ion beams. An overview of the general layout of the Purion XEmax is shown in Fig. 1. Unlike other high energy implanters, it extracts ions out of the ion source up to only charge state 3+, which increases source life by avoiding high power source operation for higher charge states. After pre-accelerating the ion beam

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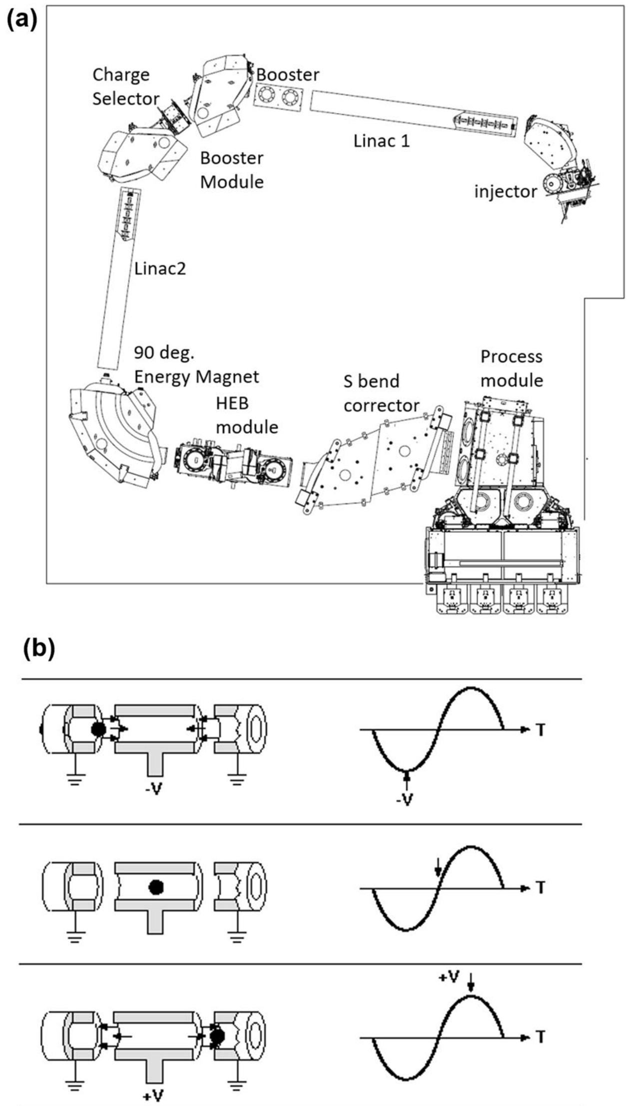

Fig. 1 **a** Schematic layout of the Purion XEmax higher energy ion implanter showing the two LINACs and Boost™ Technology which are relevant for the dataset generator. **b** Two gap RF acceleration as illustrated by one RF electrode sandwiched between two ground electrodes (left) and its voltage dependence vs time (right). For optimal acceleration a positive ion (+) will be accelerated across the first acceleration gap when the voltage reaches a minimum (pull) and vice versa for the second gap (push) as also indicated by vertical arrows on the right

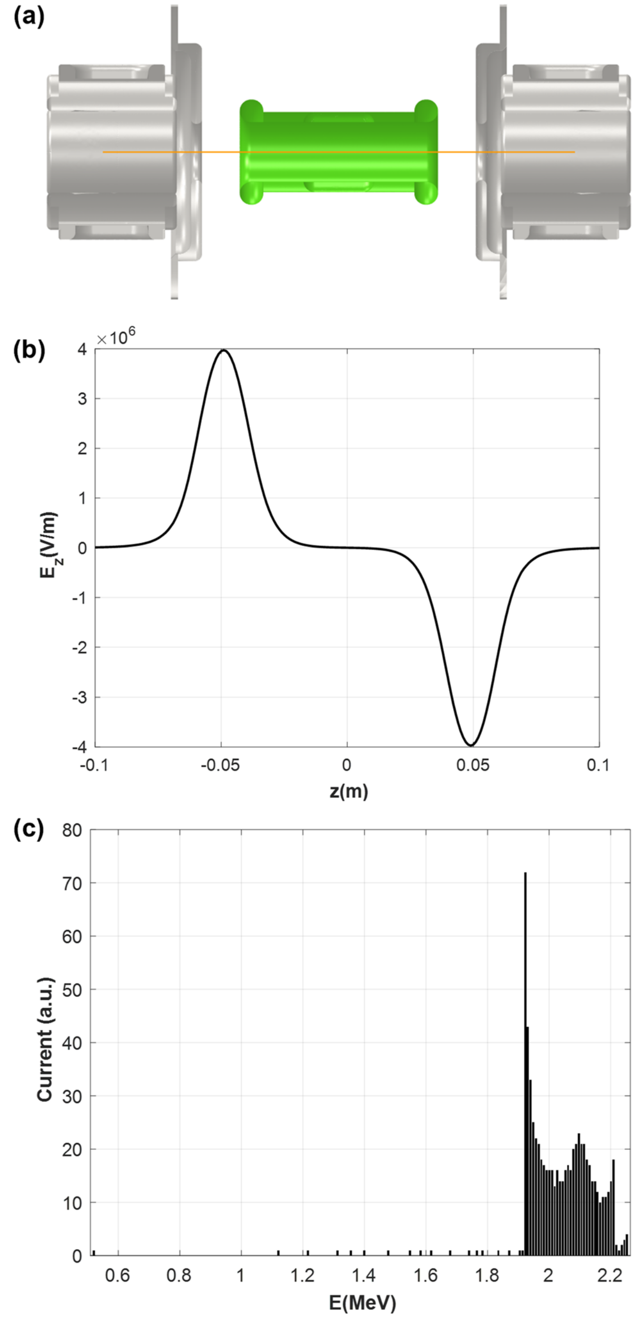

Fig. 2 **b** Electric field along center line orange line in **a**, which depicts an RF electrode (green) at − 100 kV between two electrostatic quadrupoles (gray) at ground. **c** Energy spectrum for As^{+++} accelerated with a few resonators at 13.56 MHz

with the first LINAC it utilizes Boost™ Technology to increase the charge state up to 6+. A second LINAC accelerates the ion beam to its final energy (As 15 MeV and P 14.5 MeV).

The Boost™ Technology not only enables much higher energies and beam currents with a reduced footprint (shorter LINAC), but also, by changing the charge state, it avoids possible mass-to-charge ratio (*m*/*q*) coincidences, such as $^{75}As^{++++}$ with $^{56}Fe^{+++}$, which can lead to energetic metals contamination and subsequent CMOS Image Sensor device degradation [1]. As is shown in Fig. 1a, the Purion XEmax utilizes two LINACs. Both LINACs use the pull–push acceleration scheme of a two gap resonator as schematically shown in Fig. 2. Each RF resonator is connected to an RF electrode (drift tube) which oscillates at 13.56 MHz with an amplitude on the order of 100 kV.

The challenge for optimal acceleration is to time the instantaneous position of the ions, so they cross the acceleration gaps before or after the RF electrode when the sine wave is close to a minimum (pull) or maximum (push), respectively, as shown by the position of the vertical arrow on the right of Fig. 1b. In other words, the time it takes for an ion to fly through the field free RF electrode or drift tube needs to match approximately half an RF period.

For the LINAC to be able to accelerate not only one species at a certain energy (fixed velocity profile) the phase of each resonator RF electrode can be independently varied (as well as their amplitudes). However, in order for a large number of ions to be accelerated via the pull/push scheme the continuous DC beam that gets injected from the ion source into the LINAC needs to be compressed in the longitudinal direction into small packets of beams, often referred to as bunches. This is typically accomplished with a so called buncher that operates at about 5–20% amplitude or peak voltage of all the other resonators in the LINAC. In addition, the ground electrodes that are depicted in Fig. 1b are electrostatic quadrupoles used to refocus the beam because the pull/push scheme has defocusing effects due to fringe fields as is described in various text books, for example [2, 3].

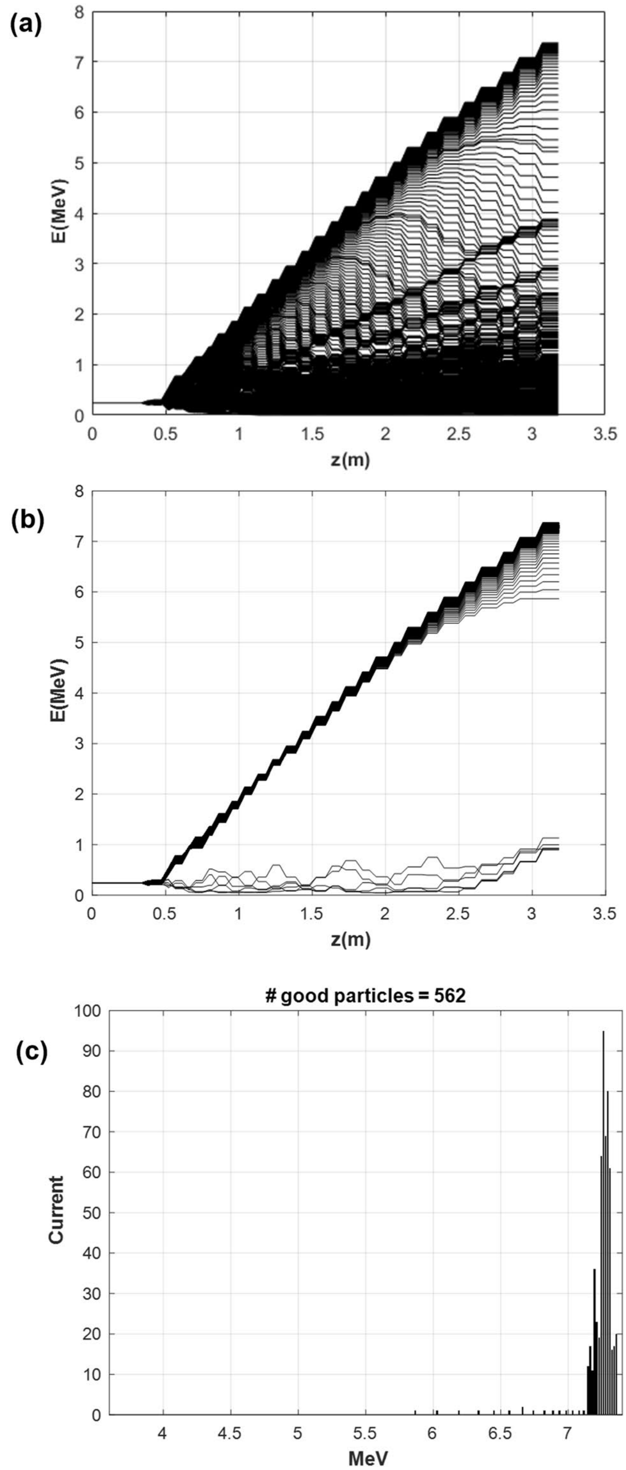

Fig. 3 Energy gain of ions as they travel through a LINAC without **a** and with zlimit removal **b** as explained in the text. **c** shows the resulting energy spectrum

Longitudinal ion dynamics code

In order to simulate the acceleration in the LINAC an in-house longitudinal ion dynamics code was written that uses the equation of motion for alternating electric fields in the RF range. Simplified non-relativistic equations are as follows:

$$F = \mathrm{ma} = m\left(d^2z/\mathrm{d}t^2\right) = qE_z$$

with $q = \mathrm{ne}$, $m = \mathrm{AMU}\ 1.66\mathrm{E}{-}27$ kg

$$a = qE_z/m$$

$$z = 0.5a\Delta t + v_0\Delta t + z_0$$

$$\Delta v = a\Delta t + v_0$$

For example, by using the electric field distribution E_z for the two acceleration gaps between an RF electrode and the preceding and succeeding electrostatic quadruples of a LINAC (Fig. 2b) the acceleration of an ion can be determined.

Instead of solving this problem analytically the 'space' z (horizontal axis in Fig. 2a) can be 'sliced' into small increments Δz. Assuming that the electric field is constant over a small space increment Δz the motion and acceleration of an ion can be stepwise calculated. If the increment Δz is sufficiently small the resulting particle motion will be quite accurate. This method is similar to what is often referred to as finite element method. Alternatively, instead of small

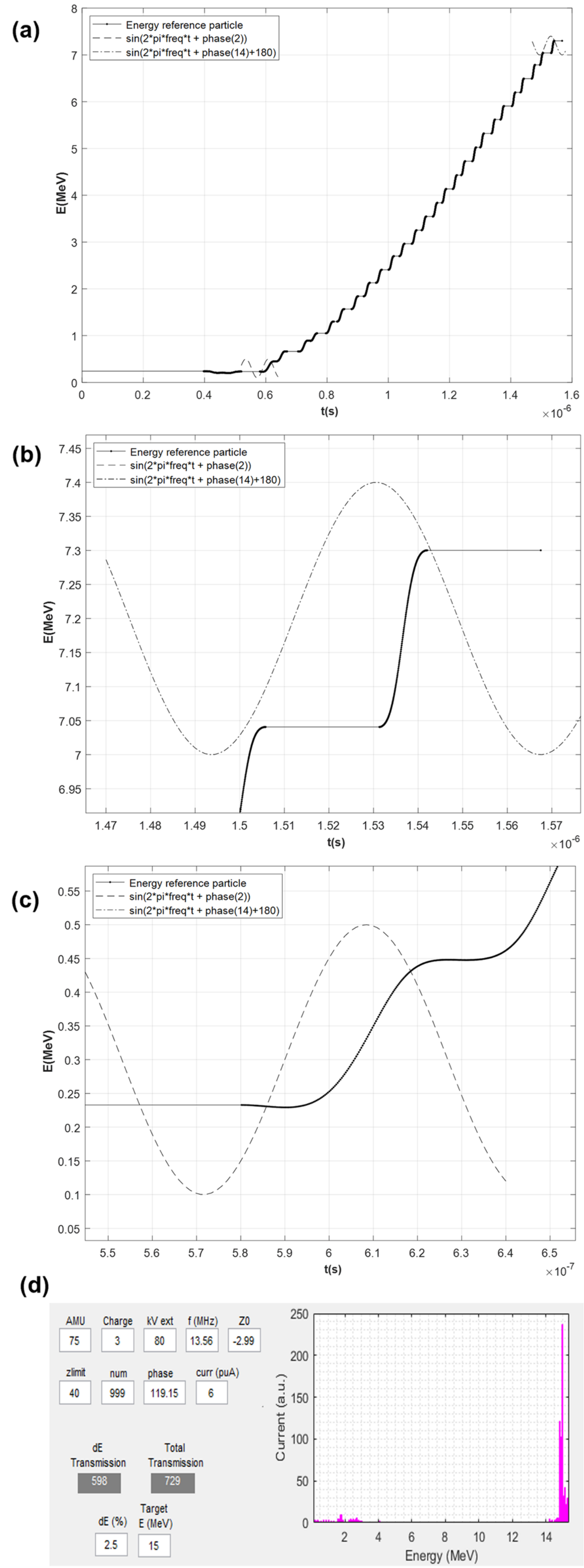

Fig. 4 **a** Energy gain of As^{+++} as it travels through a LINAC plotted vs time. For reference the variation of the RF electrode voltages are plotted to make the equivalent phase variation discernible. For better visibility **b** and **c** depict enlarged views of the data in **a** at high (**b** 7 MeV) and low energy (**c** 300–500 keV). **d** GUI excerpt showing energy spectrum for a generated dataset of As 15 MeV

increments in space Δz small increments in time Δt can be used. In addition, the electric field not only varies in space, as shown in Fig. 2b, but also in time as already discussed for Fig. 1b. One point to mention about the electric field distribution in Fig. 2b is that the fringe fields reach somewhat deep into the ground and RF electrode, so the effective gap discussed in Fig. 1b is actually larger than the geometric gap, so ions will start to get accelerated over a wider range.

This method can be applied to a LINAC with many resonators and even to multiple LINACs with other optical elements in-between such as bending magnets and quadrupoles, as well as Boost™ Technology. For simplicity the application of magnetic or electrostatic quadrupoles were left out of the description above.

When performing the simulation for many ions (for example 1000) over a time period equivalent to 360° in an RF phase a typical energy spectrum can be determined such as shown in Fig. 2c. The energy spectra look virtually identical as the ones generated by the Los Alamos' Parmela code [4].

Typically, some ions will be lost when bunching and accelerating ions by a LINAC. In Fig. 2c about 60% of the ions (transmission) were accelerated to an energy of about 2.1 MeV by using several resonators with an RF amplitude of the order of 100 kV. The RF phases were chosen carefully to maximize the energy and transmission. However, an algorithm can be employed that will determine the RF amplitudes and phases for a desired ion species and energy as will be discussed below.

Particles lagging behind the reference particle by more than typically 40 cm get lost in the beam line resulting in typical transmission of 30–50%. Therefore, a simulation parameter zlimit was defined, enabling the removal of particles which lag behind the reference particle by more than zlimit. The effect of the zlimit parameter is illustrated in Fig. 3. In Fig. 3a no particles were removed from the simulation. In Fig. 3b particles which lagged behind the reference particle by more than zlimit = 40 cm were removed from the simulation drastically reducing the total number of particles passing through the LINAC. The resulting final energy spectrum is shown in Fig. 3c.

The electric field varies as the ion gets accelerated across the acceleration gap so that the effective energy gain is reduced. This is commonly referred to as transit time factor as expressed by the Panofsky equation [3] and is most relevant for low energies. For example, as shown in Fig. 4, at low energies of 300–500 keV it can vary over 180° of equivalent phase, whereas at high energies of 7 MeV it is only about 40°. These phase changes appear larger due to the fact that the fringe fields reach somewhat deep into the RF and ground electrode as was discussed earlier for Fig. 2b.

The simulation code was written in C++ and compiled into a Dynamic Link Library (DLL). The DLL was then used in combination with a graphical user interface (GUI) written in C#, Python, and/or MATLAB. Because the code is computationally intensive this served as the fastest and most flexible option.

Dataset generator for the Purion XEmax

For optimum acceleration and transmission, the RF amplitudes, phases, and quadrupole voltages need to be chosen. However, an algorithm can be employed that will determine these parameters for a desired ion species and energy. Such an algorithm is called a dataset generator and was employed in Fig. 4d for As 15 MeV which takes into account the two LINACs and Boost™ Technology configuration of the Purion XEmax.

It determines the RF phases roughly providing a transmission of typically > 30%. As a further improvement, the phases were fine-tuned via an optimization algorithm such as the Downhill Simplex Method in multidimensions. After the fine-tuning the transmission typically improves from > 30 to > 50%, which is expected for well-tuned LINACS.

This dataset generator algorithm determines RF amplitudes that are equal for all resonators (except the buncher). This is preferable as it puts the same electrical stress on the resonators instead of stressing one resonator more than the others, which can lead to failures of the resonator components.

The dataset generator works best for a mass-to-charge ratio (m/q) for which the respective LINAC drift tubes were designed for. In some cases, the generated dataset does not provide the same transmission when applied to a real LINAC due to small mechanical differences in the LINAC structure (tolerance issues or small misalignments). However, the dataset can still serve as a starting point for further automatic tuning on the actual high-energy implanter because all that is required for implementation is that it results in some transmission at the desired energy. Typically, only ~ 5–10% transmission is sufficient since one can improve the transmission with the available standard tuning routines of the XEmax (buncher, quick or full tune).

Conclusion

A dataset generator was developed for the Purion XEmax which utilizes two LINACs and Boost™ Technology, to generate datasets for new species and/or energies quickly and efficiently. It uses an in-house written simulation code and will generate equal RF amplitudes (except for the buncher), so the electric stress on each resonator is kept to a minimum.

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Data availability The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

References

1. S. Satoh, W. Platow, S. Kondratenko, L. Rubin, P. Mayfield, R. Lessard, G. Bonacorsi, P. Whalen, R. Newman, *Purion XEmax, Axcelis Ultra High Energy Implanter with Boost Technology*, these proceedings
2. D. Boussard, Focusing in Linear Accelerators, in *Focusing of Charged Particle Beams*, vol. II, ed. by A. Septier (Academic Press, New York, 1967)
3. T.P. Wangler, *Principles of RF Linear Accelerators* (Wiley, New York, 1998)
4. L. Young, J. Billen, The Particle Tracking Code Parmela, in *Proceedings of the 2003 Particle Accelerator Conference*, 2003, p. 3521. IEEE

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