

MONTE CARLO SIMULATION ANALYSIS FOR RADIATION DAMAGE ON GLIDCOP Al-15 CAUSED BY 17-20 MeV/u HEAVY IONS*

E. Fletcher^{1†}, T. Ginter¹, P. Hurh², T. Kanemura¹, S. Lidia¹, A.S. Plastun¹, E. Wakai¹

¹Facility for Rare Isotope Beams, East Lansing, MI, USA

²Fermi National Accelerator Laboratory, Batavia, IL, USA

Abstract

The Facility for Rare Isotope Beams heavy-ion SRF linear accelerator is designed to accelerate all ions up to Uranium to a maximum beam power of 400 kW. Several beam intercepting devices are essential to the successful operation and maintenance of the accelerator, including a low power charge selector (LPCS) made of copper CONTAINING 0.15% precipitated Aluminum Oxide by weight called Glidcop Al-15. As FRIB ramps up the primary beam power beyond the current 20 kW level, the charge selector must withstand ever increasing heat loads and higher radiation damage rates. Significant beam induced radiation damage-including deformation, (e.g., swelling and blistering with cracking) has already been observed on a recently removed LPCS. We also observed physical features up to about 5.5 mm wide which appear to be deeper than the projected range of any ions.

This paper presents the results of Monte Carlo simulations carried out using the Particle and Heavy Ion Transport code System (PHITS), quantifying the total damage dose caused by ²³⁸U from 2023-2024. Simulating an accurate irradiation history is essential to determining the scope of post irradiation examination (PIE) work. This paper will also present a PIE plan in detail.

INTRODUCTION

The Facility for Rare Isotope Beams (FRIB) linear accelerator (linac) uses a charge stripper to increase the mean charge state of an ion beam, therefore increasing the energy gain of the beam from post-stripper linac cavities. This also creates multiple charge states of the beam. While the FRIB linac can simultaneously accelerate multiple charge states within a $\Delta Q/Q$ of about $\pm 3\%$, it cannot accelerate them all. The low power charge selector [1] (LPCS), as shown in Fig. 1, is a set of moving jaws that act as slits to intercept the lowest intensity charge states that cannot be accelerated and ensure that high-intensity charge states are allowed to pass through a gap between the jaws to be accelerated. This beam interception causes radiation damage due to the displacement of lattice atoms, ion implantation and other irradiation effects such as transmutation. While the effects of radiation damage are observable on the LPCS, there is little data available to show how the combined effects of

different ion species and transmutation products affect damage mechanisms.

The best place to begin understanding the complex interplay between various radiation damage effects is by looking at the contributions of individual ion species, specifically the displacement damage measured in dpa that each species causes. This information can be used to localize regions of interest to perform PIE.

This paper intends to elucidate the process by which individual ion species are evaluated for their contributions to the displacement damage using ²³⁸U as an example and explain how this information will be used to inform future PIE work.

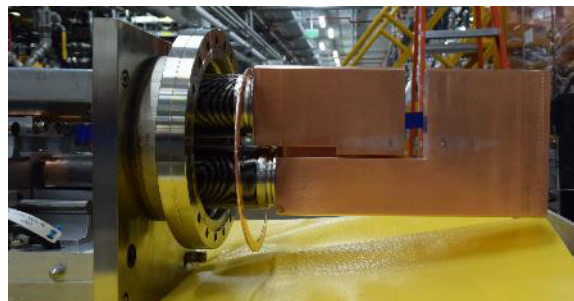


Figure 1: FRIB LPCS with visible radiation damage.

METHODOLOGY

Particle Current Calculations

To calculate the total displacement damage caused by ²³⁸U, we must first calculate the total number of particles that were intercepted by the LPCS. This must be converted from electrical current given by FRIB beam current monitors (BCMs). The conversion is given by:

$$I_p = \frac{I_{eUA}}{Q * e} \quad (1)$$

where I_p is the particle current (particles per second or pps), I_{eUA} is the charge current in electrical micro amperes, Q is the ionic charge state and e is the elementary charge. Since multiple charge states are intercepted, and each charge state only composes a fraction of the total intercepted beam, Eq. (1) becomes:

$$I_{p_i} = \frac{I_{eUA_i}}{Q_i * e} = \frac{I_{eUA} * f_i}{Q_i * e} \quad (2)$$

where f_i denotes the fraction of the contribution of a particular charge state Q_i to the intercepted beam current. Summing over the contribution of all intercepted charge states, we get:

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics and used resources of the Facility for Rare Isotope Beams (FRIB) Operations, which is a DOE Office of Science User Facility under Award Number DE-SC0023633 and Office of High Energy Physics, under Award Number DE-SC0018362.

†fletcher@frib.msu.edu

$$I_{p_{total}} = \frac{I_{euA_{total}}}{e} * \sum_i \frac{f_i}{q_i} \quad (3)$$

Measured beam current data was averaged in 6–8-hour intervals, depending on the duration of an experiment using the ^{238}U beam.

To find the total number of particles intercepted, which is necessary for the total dose calculation, simply apply Equation 3 to each 6–8-hour interval and multiply by the corresponding number of seconds in each interval. The total number of intercepted particles is the sum of the number of particles in each time interval or:

$$N_p = \sum_j I_{p_{totj}} * t_{intj} \quad (4)$$

where N_p is the total number of intercepted particles, j represents each 6-8 hour time interval, and t is in seconds.

DPA Calculations

To find the total dose delivered to the LPCS, we used the PHITS Monte Carlo code [2] to calculate the radiation damage caused by ^{238}U . A gaussian energy distribution was assumed for each charge state with a spread (σ) of 20 keV, and assuming cutoffs at $\pm 3\sigma$. However, given that the energy of each charge state is approximately the same (≈ 16.5 MeV/u), only one charge state study with PHITS is required to assess the displacement damage, as the effects of other charge states are assumed to be additive with lateral displacement from dispersion. Ten batches of 10^4 particles of the intercepted 68^+ charge state were used in the simulation for ^{238}U . Table 1 describes the relevant inputs for the PHITS simulation, including the beam energy, spot size in x (horizontal) and y (vertical), and the center position in x from the optical axis for the intercepted charge states seen in Fig. 2. The fractional contribution of each charge state is also included, as it is important in the context of Eq. (3) and the calculation to find the total dpa.

Table 1: Relevant Simulation Inputs for Intercepted Charge States of ^{238}U

Charge State	Fraction f_i	X rms (cm)	Y rms (cm)	Center Position X (cm)
68+	0.0038	0.087	0.604	-7.846
69+	0.0112	0.080	0.554	-6.718
70+	0.0343	0.073	0.497	-5.592
71+	0.1023	0.066	0.437	-4.469
72+	0.2376	0.060	0.379	-3.349
78+	0.4108	0.117	0.164	3.336
79+	0.1354	0.138	0.170	4.447
80+	0.0449	0.161	0.186	5.557
81+	0.0148	0.186	0.208	6.667
82+	0.0050	0.211	0.233	7.777

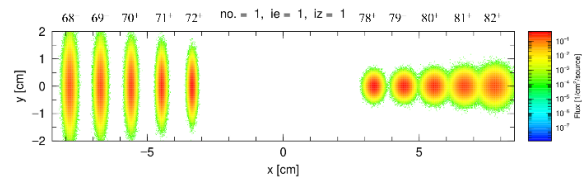


Figure 2: Intercepted charge states (top) of 17 MeV/u ^{238}U beam on the LPCS. The contours show particle flux normalized by the number of incident particles.

PHITS calculates the displacement damage rate in dpa/source, with the source being a singular particle. The displacement damage was calculated using the athermal recombination correction (arc-dpa), which corrects the standard Norgett-Robinson-Torrens dpa calculation's overestimation of the number of stable defects and underestimation of the amount of atomic mixing [3].

Once PHITS completes a simulation, the resulting dpa is output in a graph such as Fig. 3, and the peak dpa can be estimated. PHITS is also capable of calculating the dpa in the xz and yz planes, with z representing the depth of the LPCS. Since the intensity of the beam is highest in the center of the gaussian distribution, the total dpa calculation is based on the peak dpa in this region, as it is expected to be significantly larger than in the 2σ and 3σ regions of the distribution.

The resulting displacement damage rate is then multiplied by the result of Eq. (4) to find the total displacement damage.

RESULTS

Once Eq. (4) was applied to the ^{238}U current data from the years 2023-2024, the total number of particles intercepted is estimated to be $7.3 * 10^{16}$. The PHITS simulation gave the resulting displacement damage rate along the beam axis, as summarized in the Fig. 3.

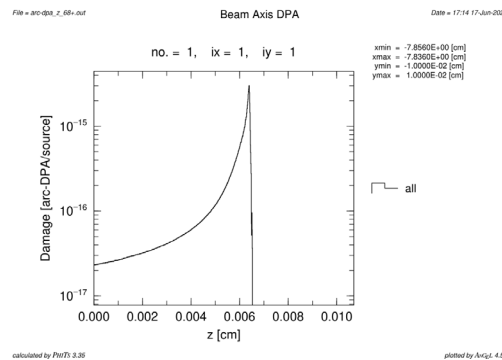


Figure 3: Arc-dpa along the beam axis near the Bragg peak.

PHITS can also calculate the displacement damage in the xz and yz planes, allowing us to approximate the dpa on the surface of the LPCS across the whole beam spot. However, the resolution is low, meaning that the error in the dpa approximation on the surface is higher than when calculating the dpa along the beam axis.

Additionally, PHITS can map the behavior of the beam, as seen in Fig. 4, allowing us to view how the beam and

secondary products such as electrons and neutrons behave as a function of depth.

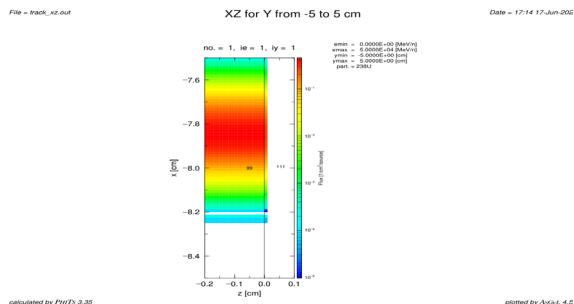


Figure 4: ^{238}U stopping behavior visualized in PHITS.

The estimated peak arc-dpa is $1.145 \cdot 10^{-15}$ arc-dpa/source with a range of 0.0065 cm. Multiplying the peak arc-dpa result by the result of Eq. (4) gives us 85.5 arc-dpa in total damage caused by ^{238}U along the beam axis over the lifetime of the removed LPCS.

DISCUSSION

While this study is limited to one singular primary beam, similar studies can be conducted in the same manner for any primary beam used at FRIB. This will allow us to create a comprehensive irradiation history for the LPCS. Compiling such a comprehensive irradiation history will inform decisions regarding the scope and breadth of current and future PIE endeavours. This methodology can also be applied to other components in the FRIB BID infrastructure such as beam dumps.

While beyond the scope of this paper, these results imply that not only can we calculate the total displacement damage, but we can also use Eq. (2) to analyze the damage per charge state as well. This would allow us to create a map of the damage across the LPCS by ion species, allowing us to determine the impact of individual ion species on radiation damage to the LPCS and other BIDs in the FRIB infrastructure, further allowing us to narrow the scope of PIE work, focusing on specific areas of interest due to ion species, amount of displacement damage and the interplay between different ion species that overlapped in the same area.

PIE Planning and Execution

FRIB is currently planning on performing PIE on the removed LPCS. As mentioned previously, it would be impractical to perform PIE on the entire affected region of the LPCS. Thus, upon visual inspection, we chose a region of particular interest as seen in Fig. 5, which appears to have sustained the most significant amount of radiation damage. This damage was likely caused by the ^{48}Ca beam. For the lifetime of the LPCS, the linac could only accelerate the 20^+ charge state of ^{48}Ca , comprising 68% of the total intensity of the beam. The damage area corresponds to approximately where the 19^+ charge state would land and contained 30% of the beam intensity with approximately 500 W of power, the maximum power for which the LPCS is rated.

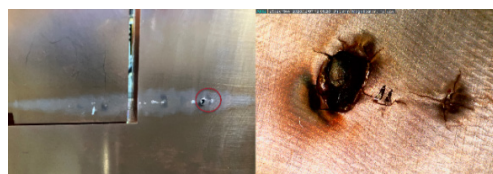


Figure 5: Damage observed on the LPCS jaw surface. The region circled in red is a zoomed in view of the region on which we intend to focus our PIE efforts.

High resolution photos of areas of high interest will be taken. A profilometer will then be used to scan the surface profile to identify areas of interest for microscopy work, and these areas will be sectioned. Once areas of interest are sectioned, SEM/EDS work will be done to find areas of high implanted ion concentration that could lead to more focused TEM work. Once optical and SEM microscopy work is complete, we will utilize nano-indentation to track the radiation hardening behavior of the material, which can help us with tracking ion diffusion into the material. Once significant areas of interest have been identified by optical microscopy and SEM, TEM imaging will be utilized to create cross-sectional images of samples. Additionally, the mechanism behind the discoloration across the LPCS as seen in Fig. 1 is unclear. Microscopy can help us determine the cause of the discoloration.

SUMMARY

Analysis of beam current data and PHITS Monte Carlo simulations allowed us to calculate the total peak displacement damage done along the beam axis by a ^{238}U beam over the lifetime of a recently removed LPCS. In addition, we were able to visualize the charge state distribution across the LPCS using PHITS and visualize the damage along the beam axis. The methods explored in this paper will allow us to perform a similar analysis for all FRIB primary beams and can be extended to any BID in the FRIB linac. Future work should explore the damage dependence on individual charge states and create comprehensive maps of the damage done by all primary beams for comparison to the observable damage on the LPCS. PIE will be performed on the LPCS to determine the interplay between various radiation damage mechanisms and a plan to do so is in effect. These simulations are the first step in correlating these effects to the displacement damage.

ACKNOWLEDGMENTS

The author would like to thank Dr. Ryoto Iwai for compiling the beam current data necessary for performing this analysis. This work was additionally supported by the Accelerator Science and Engineering Traineeship (ASET) at FRIB.

REFERENCES

- [1] A.S. Plastun *et al.*, “Advanced charge selector for stripped heavy ion beams”, in *Proc. IPAC’24*, Nashville, TN, USA, May 2024, pp. 1582-1585.
[doi:10.18429/JACoW-IPAC2024-TUPR70](https://doi.org/10.18429/JACoW-IPAC2024-TUPR70)
- [2] T. Sato *et al.*, “Recent improvements of the particle and heavy ion transport code system – PHITS version 3.33,” *J. Nucl. Sci. Technol.*, vol. 61, no. 1, pp. 127–135, Nov. 2023.
[doi:10.1080/00223131.2023.2275736](https://doi.org/10.1080/00223131.2023.2275736)
- [3] K. Nordlund *et al.*, “Improving atomic displacement and replacement calculations with physically realistic damage models,” *Nat. Commun.*, vol. 9, no. 1, p. 1084, Mar. 2018.
[doi:10.1038/s41467-018-03415-5](https://doi.org/10.1038/s41467-018-03415-5)