Exploratory study for the production of Sc beams at the ISOL facility of MYRRHA
Preliminary thermal Investigations

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Abstract

This paper reports on the start-up of an exploratory study for optimising an ISOL-target geometry towards isotopes production at driver-beam energies in the range of 100 MeV. A 1D algorithm that determines the optimal target thickness, as well as a partially algorithmic method that combines the particle-transport calculations with thermo-mechanical simulations have been developed. Further developments are planned in order to integrate an isotope-release model, as well as to provide a degree of automation, in order to facilitate optimisation. In the future this will allow easier determination of the optimal target design for the production of a specific isotope. To illustrate the optimisation process, the exploratory study for the production of scandium beams at an ISOL facility with a 100 MeV proton driver-beam is presented.

Keywords: ISOL@MYRRHA, target design, isotope production

1. Introduction

The design of high-power targets for production of Radioactive Ion Beams (RIBs) at an Isotope Separation On-Line (ISOL) [1] facility requires a full overview of the physical processes occurring in the target: nuclear reactions, thermal effects, isotope diffusion and effusion. Such targets are nowadays a requisite as they constitute one of the means to significantly increase the yields of certain RIBs to the levels required by the users. In the first phase of the MYRRHA project, the ISOL@MYRRHA [2] facility will make use of a high-power proton beam (100 MeV & 0.5 mA) in combination with high-power targets in order to produce high-intensity RIBs of various isotopes. High-power targets [3] require specific R&D to tackle engineering challenges like heat-dissipation issues while maintaining the objective of high isotope yields that are within reach with thick targets, on top of the more general considerations related to target design such as chemical reactions and release [4]. An optimisation process has been developed in order to assist with target design. In order to illustrate both the process and its potential value, we performed an exploratory study of target designs for the production of various scandium isotopes (it is important to note that the procedure can be applied to any other isotope):

- ^{41,40}Sc, which can be of interest for the physics community, as the former is a good candidate for beta decay spectroscopy [5], while the latter undergoes beta-delayed alpha and proton emission [6].
- ^{47,44}Sc, for the medical community, as they can constitute a "theranostic pair", with the former for treatment purposes and the latter for imaging [7].

So far, other facilities such as ISAC and ISOLDE have been able to produce RIBs of scandium ($^{50g\text{-}52}$Sc and $^{42\text{-}44,46\text{-}48,50,52}$Sc respectively) from metallic targets of tantalum and titanium. Some example yields:

- From ISAC, 4.1×10^5 part.s^{-1} of ^{50g}Sc from Ta target [8].
- From ISOLDE, 3×10^7 part.s^{-1}.µA^{-1} of ^{47}Sc from Ti target [9].

Note that in the case of ^{47}Sc, these quantities are orders of magnitude below what would be pre-clinically useful [7]. Furthermore, $^{41\text{-}40}$Sc have not been successfully extracted at these facilities, and it is the purpose of the present work to show how through developments in target design, these isotopes could become available.

2. Methods

Firstly, a survey of the various production routes, for the isotopes of interest, with a 100 MeV proton beam was conducted in order to determine suitable target materials from a nuclear-physics standpoint. To this end, both computed [10] and experimental [11] (when available) cross-section data for proton-induced production of scandium isotopes were compared, for several target materials, before settling on calcium and titanium as prime candidate materials (Fig. 1). As scandium is produced in both ^{44g}Sc and ^{44m}Sc forms (with ^{44m}Sc having a much longer half-life of 2.44 days), for clinical uses it is useful to know the proportion of ^{44g}Sc to ^{44m}Sc. After a hypothetical production cycle of 4 h of irradiation and 4 h for separation and transport the 44mSc activity is about 6% relative to the 44gSc activity.

Secondly, in order to gauge the optimal target thickness, a 1D optimisation algorithm was developed [12]. This algorithm computes in-target yields as a function of thickness

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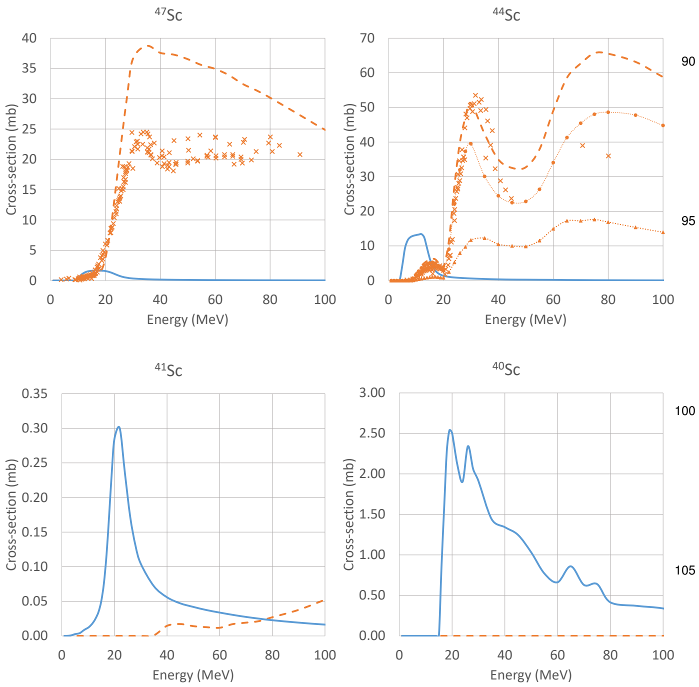

Figure 1: Proton induced cross-sections for Sc production in Ti and Ca. TENDL cross-sections from Ti are orange dashes, experimental cross-sections from natural Ti are orange crosses, TENDL cross-sections from Ca are blue lines. The dash line for ^{44}Sc cross-sections is the sum of both the ground state and metastable isotopes, whereas the line with orange circles is the ground state alone and the line with orange triangles is the metastable state alone.

using cross-section data taken from TENDL [10] and proton stopping power from TRIM [13], for specified values of incident proton current and prescribed maximum in-target power-deposition. Incident proton currents are defined as the lower value of both the maximum current available at the facility i.e. 0.5 mA and the maximum current that can be handled by an upstream proton-beam window. Note that this is a window upstream in the proton beamline with a design currently capable of handling a maximum of 0.3 mA. Maximum in-target power-deposition values are defined as the power radiated from the target container at its maximum temperature of operation, taking into account temperature limits on all other materials in the target.

Finally, the target thickness corresponding to this optimum point is then used to create a model for a full Monte Carlo simulation of the design (in FLUKA [14, 15]), where scattering and secondary production channels can be taken into account. This is essential for the subsequent thermal analysis as the heat-load distribution in the target is typically non-uniform while a uniform temperature profile is desired. The targets were irradiated with a 100 MeV proton beam uniformly distributed over the frontal surface of the target discs (diameter 4 cm). The power-deposition data resulting from the FLUKA simulation is then used as a heat-generation source for a finite-element thermo-mechanical simulation using ANSYS® Academic Research Mechanical, Release 18.0 [16]. The results of the thermo-mechanical simulation are then fed back into the FLUKA model to adjust the geometry by taking into account the thermal properties of the used materials.

The work presented here will focus on targets based on titanium and titanium-carbide. Calcium-based target materials were also examined but are not included in this contribution. Exploring materials other than the mono-atomic form allows assessing the interplay of parameters like target-element specific-density, maximum operating temperature, emissivity and conductivity, and carbide forms often have higher melting temperatures and better thermal radiation characteristics than native metallic forms.

3. Results

The obtained results are illustrated in Fig. 2. The red curves indicate the chosen current and power limitations for each combination of target material and sought isotope. The current limitation of 300 µA is determined by the aforementioned upstream proton window. The target power limitation is determined by taking the lowest value of either a simple one-dimensional calculation that takes into account the melting point (with 200 °C of margin) or the "limiting temperature" [17] (whichever is lower) of the materials in the target and the maximum power extractable from the current target container, ie. 5.5 kW. Other target containers, with increased heat-transfer capacity (using supplementary fins as in the ISAC high-power target) and other materials with higher temperature limits are being studied, hence the additional curves for higher extractable powers up to 14 kW.

Titanium has a lower melting point (1668 °C) than titanium-carbide (3140 °C and thus a lower operation temperature limit (200 °C lower than the melting temperature). However due to vaporisation/sublimation concerns in high vacuum, titanium carbide cannot be operated at temperatures near its melting point. Therefore, a "limiting temperature" of around 2000 °C in the target discs was chosen as an objective. This is why for a titanium-metal target, the maximum power to dissipate (4.8 kW) is lower than for the titanium-carbide target (5.5 kW). The intersection of the regions below a power curve and a current curve defines a permissible design region, with the maximum of that region being the optimum in terms of production. Finally, for the FLUKA and subsequent Computer-Aided Design (CAD) models used, the thickness obtained from the 1D analysis is simply divided into a number of discs, the individual thicknesses of which were determined by taking the smallest thickness values recorded in literature to be operated at ISOL facilities: 1 mm for carbide discs[18] and 20 µm for metal foils[4]. These discs have a diameter of 4 cm, in order to increase the amount of heat that can be transferred through radiative processes. When using the titanium-carbide target discs, the rest of the target is composed of a graphite hollow cylindrical container for the discs, with 2 set of graphite "windows" on either end, wrapped in a tantalum outer layer that can be used to resistively heat the target. When using the pure titanium target discs, the graphite cylinder is absent leaving only the graphite windows and the tantalum wrapper to contain the isotopes.

We performed a thermal analysis of these models, as illustrated for a titanium-carbide target in Fig. 3. The thermal distribution follows a couple of general principles: there is a radial temperature gradient, decreasing from the centre of the

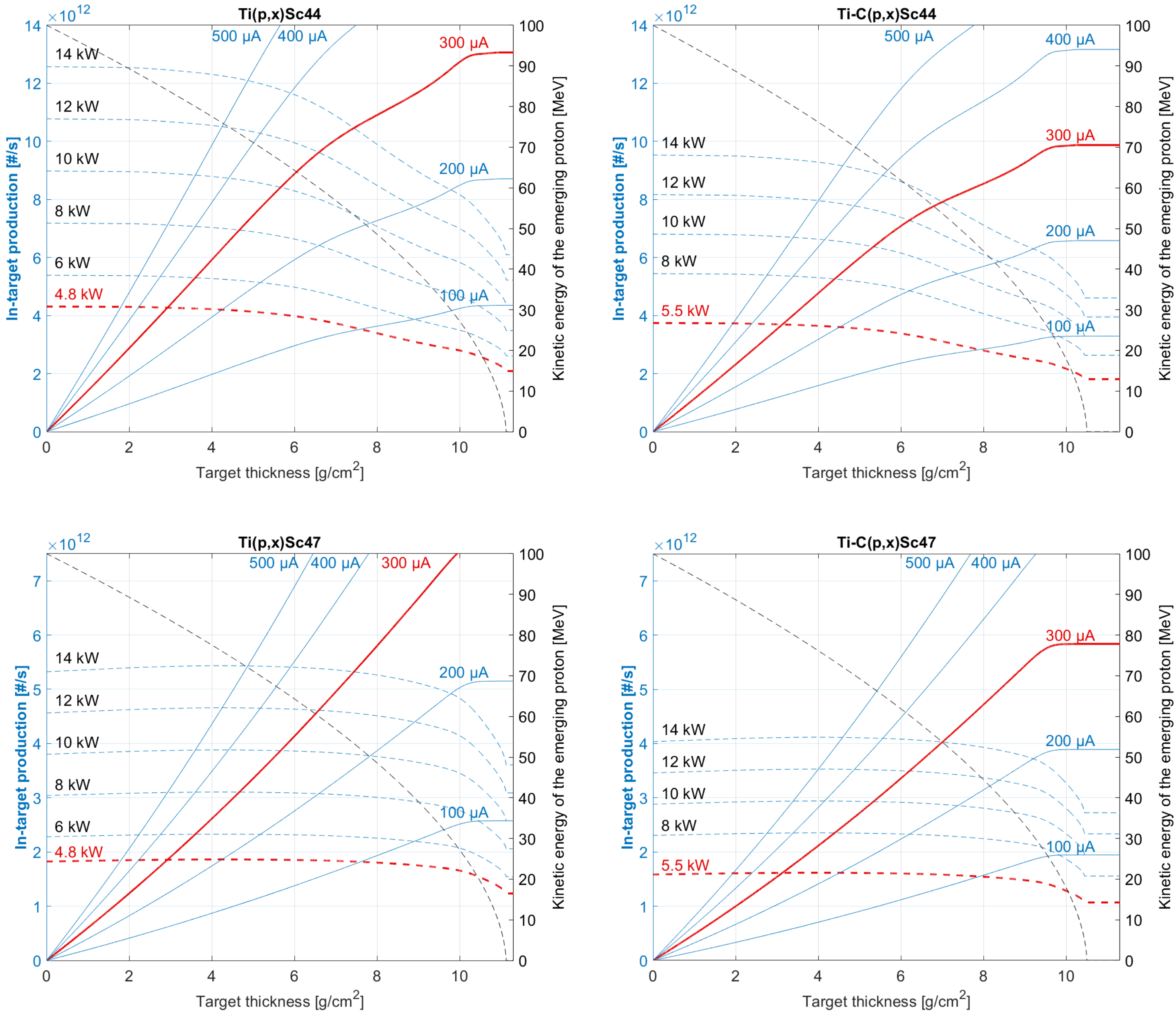

Figure 2: Results of the 1D optimisation for Ti and Ti-C using the Matlab algorithm. The blue solid and dash lines represent computed in-target production rates for different values of incident current and max power-deposition. The thickness in g/cm^2 refers to metal mass (left) and carbide mass (right). The red solid and dash lines represent respectively the reference current and power limitations currently considered for the targets. The intersection of these red lines corresponds to the optimum thickness for the target.

discs to the outer edge of the tantalum container, and there is a longitudinal non-uniformity as stopping power follows a Bragg curve as protons traverse matter (note that most of the target designs avoid reaching the Bragg peak as the heat-deposition would be very difficult to manage). Therefore, as a general rule, heat-deposition is lower where the beam enters the target and increases as protons travel towards the end, but this is of course dependent on the materials traversed, so while the heat-deposition in the exit window (leftmost side) is higher than in the entry window (rightmost side), the heat-deposition in both is much lower than in the titanium-carbide target discs. The distribution seen in the figure is that of an intermediate step in the optimisation process, and shows some of the aforementioned principles: for example, temperature tends to spike in the centres of the individual discs and the windows on either end of the target tend to be much cooler, while, longitudinally, the temperature distribution is non-uniform. Further iterations of the optimisation process are still required in order to reduce the non-uniformity in the longitudinal temperature distribution, by improving the spatial distribution of the target material discs in the target container. The addition of "buffer" graphite discs, to separate the target discs from the cold outer windows, also helps reduce the non-uniformity. The radial temperature distribution also requires some work in order to reduce the temperature gradient.

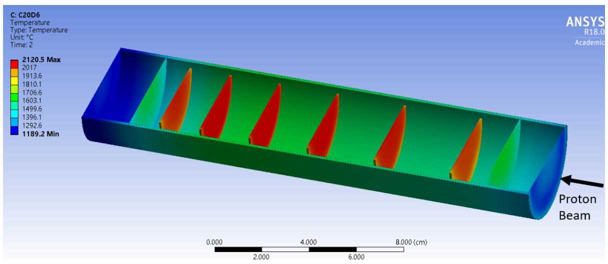

Figure 3: Example of a Ti-C target that has already undergone some rounds of optimisation in order to place the discs of target material in positions that favour a good thermal distribution. The proton beam enters from the right, and the transfer line (not shown) should be positioned halfway along the length of the target.

A thermally homogeneous target would theoretically be beneficial for the release of isotopes from the target materials: the temperature of the target should be uniformly high (hence the choice of an operating temperature as high as the material can withstand before degradation), as this usually increases diffusion speed and should also reduce the average sticking times of the isotopes on the various surfaces of the target during the effusion process. Any "cold" spots (relative to the desired operating temperature) can reduce release efficiency not only by slowing the speed of the isotopes as they migrate through matter but also by acting as "traps", where the isotopes will condense and therefore not escape the target. Finally, thermal homogeneity should also reduce thermally-induced mechanical stresses in the target. However, it is important to note that as of the time of writing, simulations of thermally-induced mechanical stresses in these target concepts are still in their early beginnings. The full study of isotope effusion and diffusion is also incomplete.

When finished, these mechanical and release simulations will also feed back into the various CAD and FLUKA models, and will form a complete optimisation procedure for the development of new targets. Experimental measurements will assist in validation of the procedure.

4. Conclusion

The concepts under investigation are an exploration of the possible optimisation routes for high-power targets. The optimisation process, in its current state of development, is a sound way of optimising target designs with respect to in-target production. However, to complete the study, release simulations complemented with more in-depth thermo-mechanical simulations have to be integrated into the optimisation process and experimental measurements are required in order to validate the process.

Acknowledgements

This work has been carried out within the scope of a PhD supported by SCK•CEN and UCLouvain.

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