Decay Characteristics of Neutron Excess Titanium Nuclei

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Abstract

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In neutron star mergers, neutron excess nuclei and the r-process are important factors governing the production of heavier nuclear systems. A single-particle model evaluation of titanium nuclei suggests that the heaviest Z = 22 nucleus will have mass 78 with filling of the $2d_{5/2}$ neutron shell. A = 62 − 78 titanium isotopes have limited experimental half-life data, but the model predicts beta decay half-lives in the range of 0.294 − 9.26 ms. Based on previous calculations for Z = 9 - 21, 26, and 30 systems and comparisons to the ^{62}Ti − ^{70}Ti calculations, summarized in the Japanese Nuclear Data Compilation, the single-particle model results likely overestimate the half-lives of A = 62 − 78 neutron excess titanium nuclei.

KEYWORDS: Nucleosynthesis, Neutron Excess Titanium Nuclei, Beta Decay, Nuclear Structure

1.0 Introduction

The nucleosynthesis of heavy elements occurs by three basic processes that add protons or neutrons to a nuclear system[1,2]. The p-process adds protons and the s- or slow process and r- or rapid process add neutrons. Capture of protons by nuclear systems produces predominantly proton-rich nuclei that tend to decay by positron emission and electron capture[1,2]. Neutron capture creates neutron-rich nuclei, and the resulting nuclear systems depend upon the rate of neutron addition and the beta decay rates of the residual nuclei.

In the s-process neutron capture chain, the time between successive neutron captures is sufficiently long for the product nucleus to beta decay to a stable system. Within the r-process, the time between neutron captures is too short to permit decays except for very rapid beta transitions. Therefore, the r-process must occur in an environment that has a high density of neutrons. For example, the s-process typically occurs in red giant stars, and the r-process occurs in a variety of astronomical events, including supernovae explosions and stellar mergers.

Binary neutron star or neutron star and stellar-mass black hole mergers can form a massive rotating torus around a spinning black hole[1]. The matter ejected from these structures and from supernovae explosions is an important source of rapid neutron capture (r-process) nucleosynthesis[1]. Fully understanding the r-process requires knowledge of the properties of neutron excess nuclei involved in creating heavy nuclear systems. Unfortunately, the majority of these

neutron excess systems have never been studied[2].

Closing this knowledge gap was a motivation for funding facilities for rare-isotope beams (FRIB) constructed at research facilities located around the world. These facilities are located at RIKEN (Japan)[3,4], GSI (Germany)[5], and Michigan State University (US)[6]. The FRIB facilities enable a new class of experiments to determine the physical properties needed by theoretical models to determine the structure of unstable neutron excess nuclei. Theoretical studies would complement experiments that provide critical information on the unstable nuclei that must be understood in order to explain nuclear abundances observed in the universe[2]. In particular, the study of neutron excess systems and their decay properties are significant considerations in understanding the r-process, and its importance in producing the observed elements in the universe.

The study of neutron excess systems is also important for determining nuclear decay properties, nuclear structure under extreme conditions, and nuclear reaction mechanisms. Existing theoretical models have not been extensively applied to many of these neutron excess nuclei.

This paper attempts to partially fill the void by calculating the decay properties of neutron excess systems that are important in nucleosynthesis. These theoretical studies should also assist in planning future experiments associated with neutron excess systems that are far removed from the line of stability.

Neutron excess nuclei that merit study occur throughout the periodic table[2-7] including nuclei in the Z ≤ 32 range[7]. Although neutron excess nuclei occur throughout the periodic table, this paper focuses on titanium systems as part of a continuing investigation of nuclei that are of potential astrophysical significance[8-22]. Previous publications addressed neutron excess calcium[8], iron[9], fluorine[10], zinc[11], neon[12], sodium[13], magnesium[14], aluminum[15], silicon[16], phosphorous[17], sulfur[18], chlorine[19], argon[20], potassium[21], and scandium[22] systems.

The study of light nuclear systems, including titanium, is important for a comprehensive astrophysical interpretation of nucleosynthesis. For example, Terasawa et al. [23] studied the role of light neutron-rich nuclei during r-process nucleosynthesis in supernovae. Specifically, Ref. 23 noted that light neutron excess systems can significantly affect the heavy-element abundances.

Recent studies emphasize the importance of studying titanium isotopes as well as their astrophysical significance[24-26]. These studies include both theoretical as well as experimental efforts, and provide additional data to assist in clarifying a picture of the evolution of nuclear structure with increasing neutron number

Refs. 24-26 have both theoretical nuclear physics as well as astrophysical importance in predicting the production of neutron excess titanium nuclei. The continuing interest in neutron excess systems suggests the importance of evaluating titanium systems considerably heavier that those investigated in Refs. 24 - 26. In particular, this paper evaluates ^{51}Ti – ^{78}Ti that span a much greater range than investigated in previous calculations.

2.0 Calculational Methodology

A variety of models could be applied to the investigation of neutron excess nuclei. These vary in sophistication, but the proposed model utilizes a basic single-particle approach. This is a reasonable first step because there are uncertainties in the nuclear potential that likely are more significant than the limitations introduced by a single-particle approach.

Since the method for calculating single-particle energies in a spherically symmetric potential is well-established only salient features are provided. The model used to describe the particle plus core system represents an application of the standard method of Lukasiak and Sobiczewski[27] and Petrovich et. al. [28]

The binding energy E_{NLSJ} of a particle in the field of a nuclear core is obtained by solving the radial Schrödinger Equation

$$\left[\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} \right) - E_{NLSJ} - V_{LSJ}(r) \right] U_{NLSJ}(r) = 0 \quad (1)$$

where r is the radial coordinate defining the relative motion of the nuclear core and the particle; $V_{LSJ}(r)$ is the model interaction; E_{NLSJ} is the core plus particle binding energy; $U_{NLSJ}(r)$ is the radial wave function; and L, S, and J are the orbital, spin, and total angular momentum quantum numbers, respectively. N is the radial quantum number, and μ is the reduced mass.

The method of searching for E_{NLSJ} is provided by Brown, Gunn, and Gould[29], and the methodology of Ref. 30 is utilized to obtain a converged solution. Refs. 8 – 22 and 28 provide a more complete description of the model, its numerical solution, and further definition of the individual terms appearing in Eq. 1.

3.0 Nuclear Interaction

Nuclear stability with respect to alpha decay, beta decay, positron decay, and electron capture is addressed using the method previously published by the author and coworkers[8-22, 28] that is similar to the approach of Ref. 31. The single-particle level spectrum is generated using a Woods-Saxon potential. Parameters of the potential are obtained from a fit to the single-particle energy levels in ^{209}Pb and ^{209}Bi performed by Rost[32]. The central potential strength of the Rost interaction[32] has a standard form and can be explicitly defined as

$$V_0 = 51.6\left[1 \pm 0.73 \frac{N-Z}{A} \right] \quad (2)$$

where the upper (lower) sign applies to protons (neutrons). The remaining parameters were held constant and are given by Rost[32]: r_0 = 1.262 (1.295) fm, r_{so} = 0.908 (1.194) fm, a = 0.70 (0.70) fm, and γ = 17.5 (28.2) for protons (neutrons) [28,32]. The spin-orbit interaction strength V_{so} is related to γ by the relationship[32]:

$$V_{so} = \frac{\gamma V_0}{180} \quad (3)$$

The scaling relationships of Eqs. 2 and 3 yield reasonable fits to observed single-particles levels in ^{120}Sn and ^{138}Ba. The pairing correction term of Blomqvist and Wahlborn[33] is used in the calculations presented herein. The pairing correction improves the predicted energies of occupied levels in ^{120}Sn, ^{138}Ba, and ^{208}Pb[28].

When applied to specific nuclei, this methodology requires modification. For example, Ray and Hodgson[34] note that ^{40}Ca and ^{48}Ca require different potentials to properly fit their single-particle level structure. Schwierz, Wiedenhöver, and Volya[35] also investigated ^{40}Ca and ^{48}Ca and noted that a proper fit to the single-particle levels required a different potential for each energy level. Difficulties in the selection of an appropriate potential is an additional motivation for the utilization of a single-particle model, and was noted in studies of neutron excess Z = 9 - 21, 26, and 30 nuclei[8-22]. Similar issues also apply to titanium systems.

In view of the results of Refs. 34 and 35, the following modification is made to obtain the titanium potential strength (V_A):

$$V_A = 51.6\lambda\left[1 \pm 0.73\frac{N-Z}{A}\right][1 \pm a(A)] MeV \quad (4)$$

where λ is a potential strength multiplier that is selected to ensure consistency with available data, and a(A) is a constant that is introduced to account for the variations in potential strength with A[34,35]. In previous neutron excess nuclei calculations for Z = 20, 26, and 30 systems[8,9,11], a value of λ = 1.0 was utilized. A λ value of 1.5 for Z = 9 – 21 systems[10,12-22] was determined by the available experimental data[36-38]. Given the proximity to the A = 21 system, a value of λ = 1.5 is also utilized for titanium. Since the paper's primary purpose is investigation of neutron excess nuclei, determining appropriate a(A) values for the heaviest titanium systems is desirable.

The heaviest mass Z = 22 isotope[36-38] suggested experimentally is ^{61}Ti. Given the expected order of energy levels, ^{61}Ti would have a partially filled $2p_{1/2}$ neutron single-particle level structure. Isotopes heavier than ^{61}Ti would require filling of the $1g_{9/2}$ and $2d_{5/2}$ neutron single-particle levels. The possibility of bound titanium isotopes with A ≥ 62 is addressed in subsequent discussion.

4.0 Calculation of Half-Lives

Using Eq. 4, single-particle levels are calculated for A ≥ 51 titanium isotopes. A ≥ 51 titanium nuclei were evaluated for stability with respect to alpha decay, beta decay, positron decay, electron capture, and spontaneous fission. These calculations were performed to ensure that the nuclear structure contained no interloping states or structural defects, and that any decay modes in conflict with data were identified.

The decay modes and half-lives of 78 ≥ A ≥ 51 titanium isotopes are summarized in Table 1, and compared to

available data[36-38] and calculations incorporated in the Japanese data compilation[38]. The alpha decay energies are calculated using the relationship based on Ref. 39

$$Q_\alpha = 28.3\,MeV - 2S_n - 2S_p \quad (5)$$

where S_n and S_p are the binding energies of the last occupied neutron and proton single-particle levels, respectively. Alpha decay half-lives can be estimated from Q_α using standard relationships[27]. Fortunately, no alpha decay modes occurred in the Table 1 summary of $78 \geq A \geq 51$ titanium isotope decay properties.

The beta decay half-lives are determined following the log ft methodology of Wong[39]. Allowed (first forbidden) transition half-lives were derived using the values of log ft = 5 (8). Given the uncertainties in the calculated level energies, second and higher order forbidden transitions were not determined. Positron and electron capture half-lives were determined following the approach of Ref. 27. Spontaneous fission half-lives are addressed using the methods noted in Refs. 40-55.

5.0 Model Issues

Spherical single-particle energy level calculations produce reasonable results for alpha, beta, positron, and electron capture transitions[8-22, 27,28], and spontaneous fission[40-55]. Neutron excess titanium isotopes also have the potential to decay via neutron emission modes. However, these decays have not been observed in titanium[36-38]. The single-particle model is not the best approach for neutron emission calculations, and these decay modes are not included in this paper. Therefore, the results for the heaviest neutron excess titanium nuclei only include the alpha decay, beta decay, positron decay, electron capture, and spontaneous fission modes. Except as noted previously, the single-particle model should provide reasonable results for the systems considered in the paper.

6.0 Results and Discussion

Using Eq. 4, the a(A) value was varied in increments of 0.0001 to assess the applicability of the proposed model to predict the decay properties of $51 \geq A \geq 78$ titanium isotopes. In view of uncertainties in the model and associated interaction, a smaller increment was not deemed to be justified.

The issues associated with fitting all Z = 9 – 21, 26, and 30 nuclei with a single potential[34,35] were noted in Refs. 8-22. These considerations are also applicable to the titanium systems considered in this paper.

Table 1 summarizes the complete set of $78 \geq A \geq 51$ titanium isotopes considered in this paper. The $78 \geq A \geq 51$ titanium isotopes fill the $2p_{3/2}$ (^{51}Ti – ^{54}Ti), $1f_{5/2}$ (^{55}Ti – ^{60}Ti), $2p_{1/2}$ (^{61}Ti – ^{62}Ti), $1g_{9/2}$ (^{63}Ti – ^{72}Ti), and $2d_{5/2}$ (^{73}Ti – ^{78}Ti) neutron single-particle levels. ^{61}Ti is the heaviest titanium system noted in Ref. 36 - 38 that has been observed experimentally. Given the extrapolation used in formulating the single-particle potential of Eq. 4, the results become more uncertain due to the paucity of data for A > 61 titanium isotopes.

Table 1 Calculated Single-Particle and Experimental Decay Properties of Titanium Nuclei with $51 \leq A \leq 78$

Nuclide	a(A)	Half-Life (Decay Mode)	
		Experiment [a,b,c]	This Work
^{51}Ti	-0.0108	5.76 min s[b]	5.72 min (β^-)[d]
^{52}Ti	-0.0182	1.7 min s[b]	1.69 min (β^-)[d]
^{53}Ti	-0.0235	32.7 s[b]	32.7 s (β^-)[d]
^{54}Ti	-0.0046	2.1 s[b]	2.11 s (β^-)[d]
^{55}Ti	-0.0580	1.3 s[b]	1.30 s (β^-)[e]
^{56}Ti	-0.0256	200 ms[b]	200 ms (β^-)[e]
^{57}Ti	-0.0134	98 ms[b]	98.0 ms (β^-)[e]
^{58}Ti	-0.0039	58 ms[b]	58.0 ms (β^-)[e]
^{59}Ti	+0.0144	30 ms[b]	30.0 ms (β^-)[e]
^{60}Ti	+0.0199	22 ms[b]	22.0 ms (β^-)[e]
^{61}Ti	+0.0309	15 ms[b]	15.0 ms (β^-)[e]
^{62}Ti	+0.0500	[f, g]	9.26 ms (β^-)[e]
^{63}Ti	+0.0637	[f, h]	6.56 ms (β^-)[e]
^{64}Ti	+0.0775	[f, i]	4.78 ms (β^-)[e]
^{65}Ti	+0.0913	[f, j]	3.57 ms (β^-)[e]
^{66}Ti	+01050	[f,k]	2.72 ms (β^-)[e]
^{67}Ti	+0.1188	[f, l]	2.12 ms (β^-)[e]
^{68}Ti	+0.1326	[f,m]	1.68 ms (β^-)[e]
^{69}Ti	+0.1463	[f,n]	1.35 ms (β^-)[e]
^{70}Ti	+0.1601	[f,o]	1.10 ms (β^-)[e]
^{71}Ti	+0.1739	[f]	0.904 ms (β^-)[e]
^{72}Ti	+0.1877	[f]	0.750 ms (β^-)[e]
^{73}Ti	+0.2014	[f]	0.630 ms (β^-)[e]
^{74}Ti	+0.2152	[f]	0.534 ms (β^-)[e]
^{75}Ti	+0.2290	[f]	0.455 ms (β^-)[e]
^{76}Ti	+0.2427	[f]	0.390 ms (β^-)[e]
^{77}Ti	+0.2565	[f]	0.338 ms (β^-)[e]
^{78}Ti	+0.2703	[f]	0.294 ms (β^-)[e]

[a]Ref. 36. [b]Ref. 37. [c]Ref. 38.

[d]Allowed $1f_{7/2}(n)$ to $1f_{7/2}(p)$ beta decay transition.

[e]Allowed $1f_{5/2}(n)$ to $1f_{7/2}(p)$ beta decay transition.

[f]No data provided in Ref. 35 - 37.

[g] The Japanese data compilation[37] notes a calculated value of 17.2 ms for ^{62}Ti.

[h] The Japanese data compilation[37] notes a calculated value of 12.5 ms for ^{63}Ti

[i] The Japanese data compilation[37] notes a calculated value of 7.69 ms for ^{64}Ti.

[j] The Japanese data compilation[37] notes a calculated value of 6.39 ms for ^{65}Ti.

[k] The Japanese data compilation[37] notes a calculated value of 4.49 ms for ^{66}Ti.

[l] The Japanese data compilation[37] notes a calculated value of 3.72 ms for ^{67}Ti.

[m]The Japanese data compilation[37] notes a calculated value of 2.53 ms for ^{68}Ti.

[n] Japanese data compilation[37] notes a calculated value of 2.14 ms for ^{69}Ti.

[o] Japanese data compilation[37] notes a calculated value of 1.62 ms for ^{70}Ti.

The neutron excess systems summarized in Table 1 were based on an evaluation of alpha, beta, electron capture, and positron decay modes. Spontaneous fission half-lives were also evaluated, but are larger that the aforementioned decay modes, particularly near closed shells.

Other decay modes that could possibly occur in neutron excess systems (e.g., n and 2n) are not readily evaluated using a single particle model, and were not evaluated. The results of Table 1 must be viewed with this limitation. However, since the neutron decay modes tend to be much shorter than the alpha, beta, electron capture, and positron decay modes[36-38], the model results provide upper bounds on the half-lives of neutron excess titanium isotopes.

6.1 51 ≥ A ≥ 61 Titanium Isotopes with Experimental Half-Life Data

The ^{51}Ti – ^{54}Ti systems fill the $2p_{3/2}$ neutron shell, and are best fit with a(A) values between -0.0235 and -0.0046 with an average value of about -0.0143. ^{55}Ti – ^{60}Ti fill the $1f_{5/2}$ neutron shell, and are best fit with a(A) values between -0.0580 and 0.0199 with an average value of about -0.0111. ^{61}Ti partially fills the $2p_{1/2}$ neutron shell, and is best fit with an a(A) value of 0.0309.

^{61}Ti is the heaviest known neutron excess titanium system. There are no experimental half-life data for A > 61 titanium systems.

The a(A) values for the ^{62}Ti – ^{78}Ti systems are based on the decreasing lifetime trends of neutron excess A = 9 – 21 systems[36-38]. Using the ^{55}Ti – ^{61}Ti values, a linear extrapolation was utilized to obtain the a(A) values for the ^{62}Ti – ^{78}Ti. The derived a(A) values are listed in Table 1.

Table 1 lists the half-life of the limiting decay transition (i.e., the transition that has the shortest decay half-life). For example, ^{56}Ti has eight beta decay transitions that are possible within the scope of the aforementioned single-particle model (i.e., allowed $1f_{7/2}$(n) to $1f_{7/2}$(p) [1.71 s], allowed $1f_{7/2}$(n) to $1f_{5/2}$(p) [1.80 h], allowed $2p_{3/2}$(n) to $2p_{3/2}$(p) [3.05 s], allowed $2p_{3/2}$(n) to $2p_{1/2}$(p) [17.9 s], allowed $1f_{5/2}$(n) to $1f_{7/2}$(p) [200 ms], allowed $1f_{5/2}$(n) to $1f_{5/2}$(p) [3.11 s], first forbidden $1d_{3/2}$(n) to $1f_{7/2}$(p) [20.9 d], and first forbidden $1f_{5/2}$(n) to $1g_{9/2}$(p) [140 d]. For ^{56}Ti the limiting beta decay mode is the allowed $1f_{5/2}$(n) to $1f_{7/2}$(p) [200 ms] transition.

As noted in Table 1, the model predicts the proper decay mode for the known 78 ≥ A ≥ 51 titanium[36-38] systems. The results for the known nuclei, summarized in Table 1, suggest that the model predictions of the neutron excess titanium systems are reasonably credible.

^{51}Ti – ^{54}Ti fill the $2p_{3/2}$ neutron shell. These systems decay via beta emission through allowed $1f_{7/2}$(n) to $1f_{7/2}$(p) transitions. Model predictions for ^{51}Ti – ^{54}Ti are within about 1% of the experimental half-lives[38]. The calculated decay modes for ^{51}Ti – ^{54}Ti are in agreement with Ref. 38.

^{55}Ti – ^{60}Ti fill the 1f$_{5/2}$ neutron shell. These systems decay via beta emission through allowed 1f$_{5/2}$(n) to 1f$_{7/2}$(p) transitions. Model predictions for the ^{55}Ti – ^{60}Ti half-lives are in agreement with the experimental half-lives[38]. The calculated decay modes for ^{55}Ti – ^{60}Ti are in agreement with Ref. 38.^{61}Ti partially fills the 2p$_{1/2}$ neutron shell. The decay mode and half-life for ^{61}Ti are in agreement with the data[38]. ^{61}Ti decays via beta emission through an allowed 1f$_{5/2}$(n) to 1f$_{7/2}$(p) transition.

6.2 78 ≥ A ≥ 62 Titanium Isotopes without Experimental Half-Life Data

The a(A) values for 62 ≥ A ≥ 78 titanium isotopeswere derived from a fit based on the half-lives of^{55}Ti – ^{61}Ti. This approach is consistent with the a(A) extrapolation methodology noted in Refs. 8 – 22. The a(A) values for 78 ≥ A ≥ 62 titanium systems are provided in Table 1.

Table 1 also summarizes calculated single-particle decay properties of titanium systems that have not yet been observed[36-38]. These systems are nuclei of interest in astrophysical applications[1-26].

The existence of 78 ≥ A ≥ 51 titanium systems, as predicted by the proposed model, is dependent on the characteristics of the interaction of Eq. 4. Although the existence of some of these systems may be an artifact of the model interaction, their study is of critical importance in understanding the role of neutron excess titanium systems in nucleosynthesis.

The ^{62}Ti system completes filling of the 2p$_{1/2}$ neutron shell, and has a beta decay half-live of 9.26 ms. This system decays through an allowed 1f$_{5/2}$(n) to 1f$_{7/2}$(p) beta decay transition. Japanese Data Compilation calculations[38] for ^{62}Ti is consistent with the model results. The ^{63}Ti – ^{72}Ti systems fill the 1g$_{9/2}$ neutron shell.

These systems decay through an allowed 1f$_{5/2}$(n) to 1f$_{7/2}$(p) beta decay transition. The ^{63}Ti – ^{72}Ti half-lives decrease from 6.56 to 0.750 ms, respectively. Japanese Data Compilation calculations[38] for ^{63}Ti – ^{72}Ti are also consistent with the model results.

The ^{73}Ti – ^{78}Ti systems complete filling the 2d$_{5/2}$ neutron shell. These systems decay through an allowed 1f$_{5/2}$(n) to 1f$_{7/2}$(p) beta decay transition. The ^{73}Ti – ^{78}Ti half-lives decrease from 0.630 to 0.294 ms.

No titanium systems with A > 78 are predicted by the model. This occurs because the 2d$_{5/2}$ neutron single-particle level is the last bound neutron state, and only 56 neutrons are bound in titanium systems. However, in view of the model potential uncertainties, the calculated properties of the heaviest titanium systems summarized in Table 1 are not definitive.

The predicted A = 62 – 78 titanium isotopes have no experimental data, but the model predicts beta decay half-lives in the range of 0.294 – 9.26 ms. Based on calculations in Z = 9 - 22, 26, and 30 systems[8-22] and calculations summarized in the Japanese Data Compilation[38], the results summarized in this paper likely overestimate the beta decay half-lives of A = 62 – 78 neutron excess titanium nuclei. The model results are also likely to be an overestimate of the half-lives because the single-particle level calculations do not evaluate the short-lived neutron decay modes in the A = 62 – 78 titanium

nuclei.

7.0 Conclusions

Single-particle level calculations suggest that neutron excess titanium isotopes terminate with^{78}Ti and filling of the $2d_{5/2}$ neutron single-particle level. The $62 \leq A \leq 78$ titanium systems have predicted beta decay half-lives in the 0.294 – 9.26 ms range, and likely overestimate the actual half-life values.

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