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Coexisting shapes with rapid transitions in odd-Z rare-earth proton emitters

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The phenomenon of shape coexistence and rapid shape phase transitions expected in deformed odd-Z proton emitters from $Z = 51$ to 75 are investigated using the triaxially deformed Nilsson potential and Strutinsky's prescription for the evaluation of shell correction. Calculations suggest prolate and triaxial shapes with large deformations except for a few oblate deformations, along with the occurrence of some coexisting configurations with different intrinsic shapes. Shape coexistence is observed in ^{113}Cs with two energy minima for different shapes at similar energies. Location of the first proton unbound nuclei for odd-Z rare-earth region is predicted and compared with the available experimental data.

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I. INTRODUCTION

Decay by spontaneous proton emission from proton-rich nuclei [1] in ground states or isomeric states has attracted lot of attention in recent times as it can be used as a powerful tool to probe the structure of proton unbound Nilson orbitals and investigate nuclear deformations beyond the proton drip line. Experimental advances in measuring proton decay and identification of a large number of ground-state and isomeric excited-state proton emitters [2–4] near the proton drip line require reliable theoretical predictions to interpret the experimental data as well as to provide guidance and valuable input into future experiments.

So far ground-state proton radioactivity has been reported for odd-Z nuclei mainly in the mass regions $51 \leqslant Z \leqslant 55$ and $69 \leqslant Z \leqslant 83$ as for nuclei with $Z > 50$, the relatively high potential energy barrier causes nuclei to survive long enough to be detected experimentally [4]. Spectroscopy of proton emitters $Z \leqslant 69$ with the discovery of proton radioactivity from the rare-earth region nuclei ^{131}Eu and ^{141}Ho [5,6] and proton decay rates of ^{109}I and ^{112,113}Cs [7–12] nuclei indicate large deformations. Lifetimes of deformed [13,14] proton emitters provide information on the last occupied Nilson configuration and hence the shape of the nucleus, which is one of the most fundamental properties of the atomic nucleus. Nuclear shapes are very sensitive to structural effects and can change with isospin and from one nucleus to its neighbor. In light nuclei ($Z, N < 40$), one finds that the ground-state prolate and oblate shapes occur more or less equally but for N, $Z > 50$ the prolate shapes are more probable [15] where the shell structure has changed from a harmonic oscillator type to a Mayer-Jensen type with a high-j intruder orbital in each major shell. Oblate shapes are expected to occur just below the $N = 82$, 126 and $Z = 82$ shell closures due to the strong shape-driving effect of holes in the $\Omega = 1/2$ orbitals [16]. In some cases configurations corresponding to different shapes may coexist at similar energies, which may be understood as arising from intruder excitations [17], in particular at and near closed-shell regions due to occurrence of many-particle–many-hole excitations across shell gaps, which may become energetically favorable at particular nucleon numbers as a result of the interplay between shell effects and the neutron-proton interaction [18].

To look for rapid shape phase transitions and shape coexistence in the ground state of highly deformed proton-rich rare-earth-region nuclei is the aim of present work. Theoretical predictions of strongly deformed prolate and few oblate shapes in $Z > 50, N < 82$ region within the Hartree-Fock-Bogoliubov (HFB) framework [15] with Gogny D1S interactions [19] and rapid shape transitions from $N < 78$ to $N > 82$ using relativistic mean field (RMF) calculations [20] show that the neutron-deficient rare-earth nuclei represent an interesting region to explore the rapidly changing shapes [15,20,21] with large deformation and the possibility of interesting phenomena of shape coexistence [17,22–27], which obviously needs a detailed investigation on theoretical as well as experimental fronts.

In this article, I present results of a thorough investigation of nuclear shapes, deformations, and the phenomenen of shape coexistence in the whole chain of neutron-deficient isotopes of rare-earth odd-Z nuclei from $Z = 51$ to 75. Observation of shape coexistence in this region is one of the main highlights of the present work. Although various mean field theories [15,20] are being used to understand structural transitions in the nuclei, the macroscopic-microscopic formalism provides in its own way a simplistic and effective approach to trace structural aspects and precise positions of proton drip lines close to the $N = Z$ line. Moreover, I also include triaxial shapes in my calculations in addition to axially symmetric shapes. Calculations are performed within the framework of triaxially deformed Nilsson potential including shell corrections where the classical collective properties of the liquid drop model are combined with the quantum corrections due to shell effects via Strutinsky formalism [28] by incorporating higher order corrections with Hermite polynomials. Energy minima are searched for Nilsson deformation parameters β and γ, where I find various γ competing for E minima, which sometimes leads to a situation where E minima are found to coexist for two γs with similar energies.

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II. THEORETICAL FORMALISM

Shapes of the atomic nuclei are governed by delicate interplay of macroscopic bulk properties of nuclear matter and the microscopic shell effects, which are treated with Nilsson-Strutinsky prescription, which starts with the well-known Strutinsky density distribution function [28–30] for single-particle states

$$g(\tilde{\epsilon}) = \frac{1}{\sqrt{\pi}\gamma} \sum \exp(-u_i)^2 \sum_{k=0}^{\infty} C_k H_k(u_i), \qquad (1)$$

where

$$u_i = \frac{(\epsilon - \epsilon_i)}{\gamma}, \qquad (2)$$

and the coefficients C_k are

$$C_k = \begin{cases} \frac{-1^{k/2}}{2^k (k/2)!} & k \quad \text{even}, \\ 0 & k \quad \text{odd}. \end{cases} \qquad (3)$$

Hermite polynomials $H_k(u_i)$ up to higher order of correction ensure smoothed levels. The energy due to Strutinsky's smoothed single-particle level distribution is given by

$$\tilde{E} = \int_{-\infty}^{\mu} \tilde{g}(\epsilon) d\epsilon. \qquad (4)$$

The chemical potential μ is fixed by the number-conserving equation

$$N = \int_{-\infty}^{\mu} \tilde{g}(\epsilon) d\epsilon. \qquad (5)$$

The shell correction to the energy is obtained as usual,

$$\delta E_{\text{Shell}} = \sum_{i=1}^{A} \epsilon_i - \tilde{E}, \qquad (6)$$

where the smearing width of 1.2 $\hbar\omega$ has been used. The single-particle energies ϵ_i as a function of deformation parameters (β, γ) are generated by Nilsson Hamiltonian for the triaxially deformed oscillator diagonalized in a cylindrical representation [31,32]:

$$H = p^2/2m + (m/2)\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right) + C\mathbf{l}\cdot\mathbf{s} + D(\mathbf{l}^2 - 2\langle \mathbf{l}^2 \rangle). \qquad (7)$$

The coefficients for the $\mathbf{l}\cdot\mathbf{s}$ and $\mathbf{l}^2$ terms are taken from Seeger [33], who has fitted them to reproduce the shell corrections [28] to ground-state masses. Strutinsky's shell correction δE_{Shell} added to macroscopic binding energy of the spherical drop B_{LDM} [34] along with the deformation energy E_{def} obtained from surface and Coulomb effects gives the total binding energy B_{gs} as in my earlier works [35,36] corrected for microscopic effects of the nuclear system:

$$B_{gs}(Z,N,\beta,\gamma) = B_{\text{LDM}}(Z,N) - E_{\text{def}}(Z,N,\beta,\gamma) - \delta E_{\text{shell}}(Z,N,\beta,\gamma). \qquad (8)$$

Energy $E(= -B)$ minima are searched for various β (0 to 0.4 in steps of 0.01) and γ [from -180° (oblate) to -120° (prolate) and $-180^\circ < \gamma < -120^\circ$ (triaxial)] to trace the nuclear shapes and equillibrium deformations. The precise position of the first unbound proton is located by one proton separation energy approaching zero value obtained as the difference between the binding energies B_{gs} of the parent and daughter nucleus. My calculated values show good agreement with the available experimental data [37] and the recent data on proton radioactivity from proton emitters ^{131}Eu, ^{141}Ho [5], and ^{145,147}Tm [9,38] lying beyond the drip line.

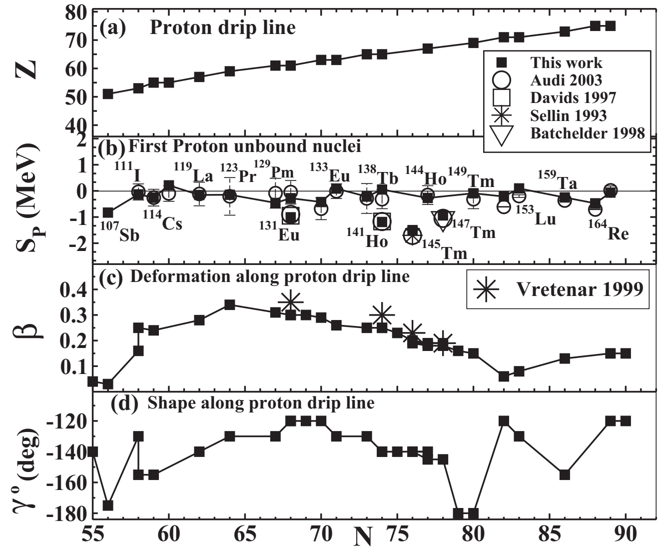

FIG. 1. Z vs N locating precise position of proton drip line for odd Z (=51 to 75) nuclei of rare-earth region. (b) $1P$ separation energy vs N for first proton unbound nucleus with $S_P \leqslant 0$ along with experimentally predicted proton drip line [37]. In addition, S_P of experimentally identified proton emitters ^{131}Eu, ^{141}Ho [5], and ^{145,147}Tm [9,38], which are in close agreement with my calculated values, are also shown. (c) Deformation parameter β vs N along my predicted proton drip line shown in panels (a) and (b). Self-consistent ground-state quadrupole deformations [39] for experimentally identified proton emitters ^{131}Eu, ^{141}Ho, and ^{145,147}Tm are also shown. (d) Shape parameter γ vs N along my predicted proton drip line of panels (a) and (b).

III. RESULTS AND DISCUSSION

The precise position of the proton drip line nuclei for odd Z from 53 to 75 in the rare-earth region is traced in Fig. 1(a). Figure 1(b) shows my calculated values of $1p$ separation energy S_P as a function of neutron number N for nuclei lying on or beyond the proton drip line, which show very good agreement with the experimental values [37]. The first proton unbound nuclei with $S_P \leqslant 0$ defining the proton drip line are predicted to be ^{111}I, ^{114}Cs, ^{119}La, ^{123}Pr, ^{129}Pm, ^{133}Eu, ^{138}Tb, ^{144}Ho, ^{149}Tm, ^{153}Lu, ^{159}Ta, and ^{164}Re, displayed in Fig. 1(b), which are in good agreement with the experimental data [37] and better than the theoretical [34] prediction of drip line except for nuclei Cs, Pm, Eu, Tb, and Lu, where the position of the drip line differs by one neutron number, although the calculated values of proton separation energy lie close to experimental values well within the error bars. Experimentally identified proton emitters ^{131}Eu, ^{141}Ho [5], and ^{145,147}Tm [9,38] lying

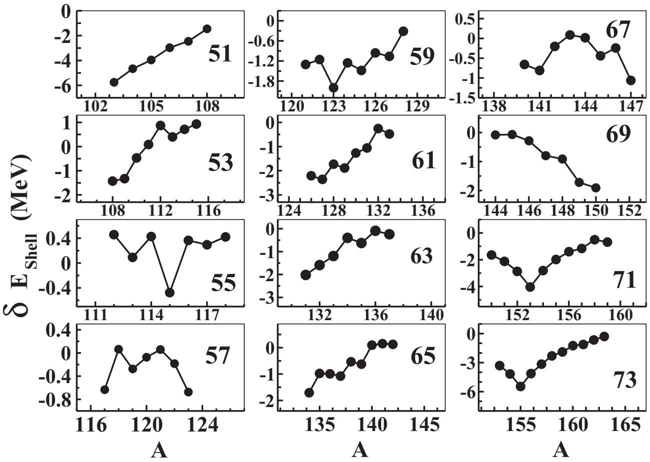

FIG. 2. Variation of shell correction $\delta E_{\rm Shell}$ values (in MeV) with A is shown for $Z = 51$ to 73.

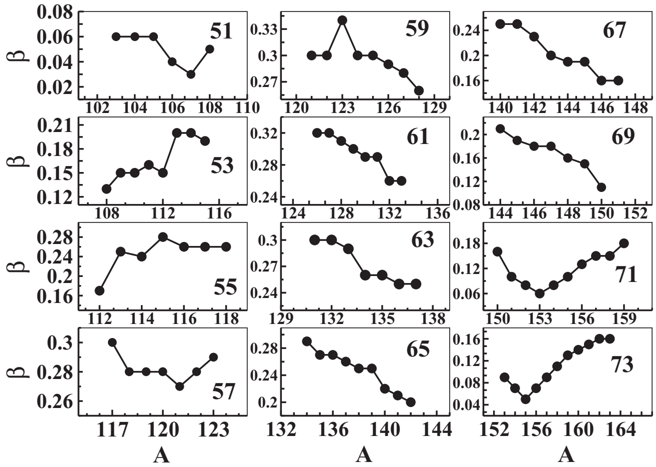

FIG. 3. β vs A for neutron deficient isotopes of odd Z (= 51 to 73).

beyond drip line are also displayed in Fig. 1(b) and show excellent agreement with my values. Proton drip lines ^{124}Pr, ^{129}Pm, ^{134}Eu, ^{139}Tb, ^{146}Ho, and ^{152}Tm within the relativistic Hartree-Bogoliubov (RHB) framework [39] for odd-Z nuclei $59 \leqslant Z \leqslant 69$ are also quite close except for Ho and Tm.

The experimental observables most closely related to the nuclear shape are quadrupole moments of excited states, and electromagnetic transition rates between them and their measurements to study [17,27] shapes and shape coexistence provide impetus to theorists to test their nuclear structure model predictions. I locate energy minima with respect to Nilsson deformation parametrs (β, γ) and present for the first time a complete trace of equillibrium deformations and shapes along the proton drip line in an odd-Z rare-earth region yet unexplored fully. Figures 1(c) and 1(d) show β and γ plotted as function of N for proton unbound nuclei predicted in Fig. 1(b). Proton emitters in this region are found to be strongly deformed with β up to $\geqslant 0.3$ except near shell closure $Z = 50$ and $N = 82$. The shapes along the drip line turn out to be mostly triaxial with some prolate and very few oblate shapes in contrast to the predicted [15,39] prolate dominance for $N, Z > 50$. However, the occurance of few oblate shapes near $N = 78$ while approaching shell closure agrees with the Refs. [15,39]. Self-consistent ground-state quadrupole deformations [39] for experimentally identified proton emitters ^{131}Eu, ^{141}Ho, and ^{145,147}Tm are close to my values, as seen in Fig. 1(c).

An estimate of the values of shell correction to energy of the ground-state odd-Z (=51 to 73) proton emitters is presented in Fig. 2. Shell correction to energy $\delta E_{\rm shell}$ varies from approximately -7 MeV (near closed shells $N = 50$, 82) up to a few keV towards the midshell nuclei, which point towards the shape transitions from near spherical to highly deformed, as is also indicated in Refs. [5,40] that the nuclei with $51 \leqslant Z \leqslant 55$ and $69 \leqslant Z \leqslant 83$ are nearly spherical whereas nuclei below $Z = 69$ are expected [6] to be strongly deformed because the proton decay rates showed significant deviations from the calculations assuming spherical basis. It is quite evident that for the spherical systems, orbital angular momentum l is a good quantum number and proton decay rates sensitive to l of the emitted proton are in general well reproduced within the spherical picture [4,5,40], though there were certain exceptions for ^{109}I and ^{112,113}Cs [7–12], which showed moderate deformations and need a thorough probe. Experimental observation of proton emission from a short-lived isomeric state of ^{141}Ho at about 60 MeV excitation energy [41] and speculation of quadrupole deformation of $\beta_2 \approx 0.23$–0.24 in subsequent works [42–44] open up a new front for research on proton-decaying excited states with large deformation, which will be discussed in my subsequent work, as done earlier [35,45].

A complete set of evaluated values of β and γ for the whole series of neutron-deficient odd-Z nuclei in the rare-earth region is presented in Figs. 3 and 4. In the proximity of the shell closure $Z, N = 50$, the deformation is very small for Sb isotopes and the shape is mostly triaxial and oblate near the closed shell. As expected the rapid shape transitions [15,20,21] are seen from oblate ($\gamma = -180^\circ$) at ^{103}Sb to triaxial ($\gamma = -145^\circ$) at ^{104}Sb to nearly prolate ($\gamma = -130^\circ$) at ^{105}Sb and then again to triaxial to oblate as I move to higher

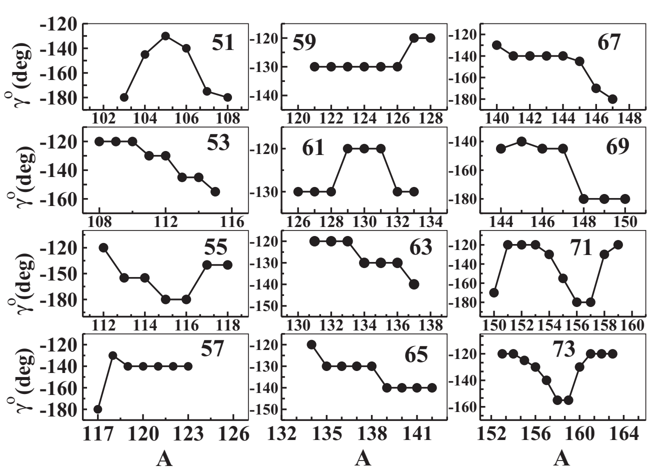

FIG. 4. γ vs A for neutron-deficient isotopes of odd Z from 51 to 73.

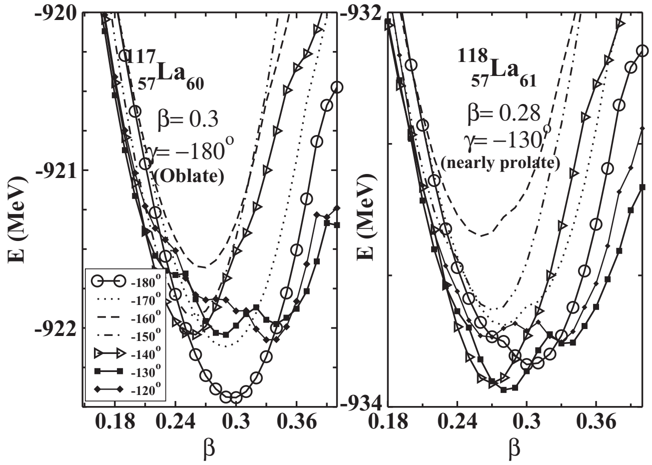

FIG. 5. Energy minimization curves with β and γ for ^{117}La and ^{118}La. Various γs are seen competing very closely for energy minima.

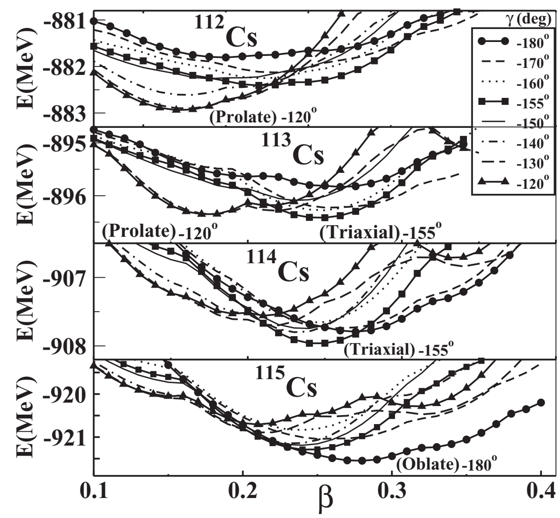

FIG. 6. Energy minimization curves with β and γ showing shape transitions in ^{112,113,114,115}Cs. Two energy minima are seen in ^{113}Cs, showing shape coexistence.

N. With increasing Z, the deformed prolate ($\gamma = -120^\circ$) shapes are seen for the most proton-rich isotope and then with increasing N, transition to triaxial ($^{113-115}$I, ^{113,114}Cs) and few oblate (^{115,116}Cs and ^{117}La) shapes are observed. β gradually increases from values 0.12–0.2 for $^{108-115}$I to $\beta \approx 0.16$–0.28 for $^{112-118}$Cs up to $\beta \approx 0.3$ in La isotopes. The interesting feature of this investigation is that the most neutron-deficient isotopes of $Z = 59$ (Pr), 61 (Pm), 63 (Eu), and 65 (Tb) are most strongly deformed with β reaching up to 0.3–0.34 and have more prolate or nearly prolate shapes, which undergo a shape transition to triaxial as the neutron number increases. As one moves toward higher $Z = 67$ (Ho), one can see in Fig. 3 that the β values start reducing to lower values of the order of 0.15 and then reduces to further lower values as one moves towards $N = 78,80$ while approaching the shell closure $N = 82$. Deformations substantially reduce to very small values near the shell closure $N = 82$ in Tm ($Z = 69$), Lu ($Z = 71$), and Ta ($Z = 73$) isotopes. Also it should to be mentioned that there is a slight deviation in my predicted β values from those of Vreterner *et al.* [39]. This could be due to inclusion of triaxiality in my calculations, whereas Vretener *et al.* [39] have considered only prolate and oblate shapes, and since many nuclei in this region are found to exhibit triaxial shapes, this justifies the slight deviation in values.

Energy minimization with β and γ is shown for ^{117,118}La in Fig. 5. A rapid shape change takes place from oblate shape in ^{117}La to nearly prolate in its neighboring isotope ^{118}La. Oblate and prolate shapes appear to coexist within an energy interval of ≈200 keV but as Fig. 5(a) suggests that the oblate shape stands out with a well-defined minima in ^{117}La. In ^{118}La, $\gamma = -130^\circ$ (nearly prolate) attains energy minima although other γ values -140° (triaxial) and -180° (oblate) are competing closely for energy minima within an energy interval of few keV.

The phenomena of shape coexistence with rapid shape transitions is displayed in the Fig. 6 with the energy minimization curves of neutron-deficient nuclei ^{112,113,114,115}Cs. These nuclei are expected to be deformed as pointed out by experiments on transitional nuclei ^{112,113}Cs [7,9,11] with emphasis on the need of calculations including deformation parameter β [46,47]. The deformation parameter $\beta = 0.17$ in ^{112}Cs increases up to $\beta = 0.28$ at ^{115}Cs with a shape change from prolate (^{112}Cs) to triaxial (^{113,114}Cs) to oblate (^{115}Cs) but the most striking feature is the coexisting prolate and triaxial shapes at ^{113}Cs. During the smooth transition from prolate shape at ^{112}Cs to triaxial ($\gamma = -155^\circ$, $\beta = 0.24$) at ^{114}Cs, one observes shape coexistence at ^{113}Cs where both prolate ($\gamma = -120^\circ$, $\beta = 0.17$) and triaxial ($\gamma = -155^\circ$, $\beta = 0.25$) shapes are coexisting at similar energies, and hence two energy minima are seen in ^{113}Cs. Further moving to higher N, the shape transition from triaxial to well-deformed ($\beta = 0.28$) oblate shape at ^{115}Cs takes place.

IV. CONCLUSION

Ground-state proton emitters in the rare-earth region with odd Z from 51 to 75 are investigated to look for rapid shape transitions and shape coexistence expected in this region. Equillibrium deformation and shapes are evaluated for the whole chain of neutron deficient isotopes of odd-Z (= 51 to 75) nuclei. Proton emitters $51 \leqslant Z \leqslant 55$ and $69 \leqslant Z \leqslant 83$ have moderate deformations with more of triaxial shapes with few prolate and oblate deformations, whereas nuclei $57 \leqslant Z \leqslant 67$ are strongly deformed with β up to 0.3–0.34 with prolate dominance in particular in Pr, Pm, Eu, and Tb nuclei with transition to triaxial shapes with higher N. The region explored here is γ soft and various γ compete closely for energy minima, sometimes leading to coexisting configurations at similar energies as seen in ^{117,118}La and $^{112-115}$Cs. The phenomenon of shape coexistence is observed in ^{113}Cs where prolate and triaxial shapes coexist with strong deformations. Proton drip line in the rare-earth region with odd-Z is predicted, which compares well with the available data. Nuclear shapes and deformation along this drip line are traced.

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