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A study on nuclear properties of Zr, Nb, and Ta nuclei used as structural material in fusion reactor

Halide Sahan[1,a], Eyyup Tel[1], Muhittin Sahan[1], Abdullah Aydin[2], Ismail Hakki Sarpun[3], Ayhan Kara[4] and Mesut Doner[1]

[1]*Osmaniye Korkut Ata University, Faculty of Arts and Science, Department of Physics, Osmaniye, Turkey*
[2]*Kirikkale University, Faculty of Arts and Science, Department of Physics, Kirikkale, Turkey*
[3]*Afyon Kocatepe University, Faculty of Arts and Science, Department of Physics, Afyonkarahisar, Turkey*
[4]*Sinop University, Faculty of Engineering, Department of Nuclear Energy Engineering, Sinop, Turkey*

Abstract. Fusion has a practically limitless fuel supply and is attractive as an energy source. The main goal of fusion research is to construct and operate an energy generating system. Fusion researches also contains fusion structural materials used fusion reactors. Material issues are very important for development of fusion reactors. Therefore, a wide range of fusion structural materials have been considered for fusion energy applications. Zirconium (Zr), Niobium (Nb) and Tantalum (Ta) containing alloys are important structural materials for fusion reactors and many other fields. Naturally Zr includes the ^{90}Zr (%51.5), ^{91}Zr (%11.2), ^{92}Zr (%17.1), ^{94}Zr (%17.4), ^{96}Zr (%2.80) isotopes and ^{93}Nb and ^{181}Ta include the ^{93}Nb (%100) and ^{181}Ta (%99.98), respectively. In this study, the charge, mass, proton and neutron densities and the root-mean-square (rms) charge radii, rms nuclear mass radii, rms nuclear proton, and neutron radii have been calculated for $^{87\text{-}102}$Zr , ^{93}Nb,^{181}Ta target nuclei isotopes by using the Hartree–Fock method with an effective Skyrme force with SKM*. The calculated results have been compared with those of the compiled experimental taken from Atomic Data and Nuclear Data Tables and theoretical values of other studies.

1 Introduction

There are many advantages of the fusion energy system. One of the most important advantages is the abundant fusion fuel availability in the nature, contrary to relatively scarce fission fuel resources. Fusion-based nuclear power experiments attempt to create similar conditions using less dramatic means, although to date these experiments have failed to maintain conditions needed for ignition long enough for fusion to be a viable commercial power source.

The success of fusion power system is dependent on performance of the first wall, blanket or divertor systems [1]. In design of a fusion reactor, one of the most important parameters is the selection of the suitable structural material to improve its neutronic performance. The performance of structural materials for fusion power systems and understanding nuclear properties are important. The Hartree-Fock method with an effective interaction with Skyrme forces is widely used for studying the properties of nuclei [2-5]. This method allows possibility to calculate many aspects of nuclei by means of quantum mechanical methods in microscopic scale [6,7]. Especially, the method is successfully used for a wide range of nuclear characteristics such as binding energy, rms charge radii, neutron and proton density, electromagnetic multipole moments, etc. In this paper, rms charge, mass, neutron, proton radii, and charge, mass, neutron, proton densities were calculated by using the Hartree-Fock method with an effective interaction with Skyrme forces for the $^{87\text{-}102}Zr$, ^{93}Nb,^{181}Ta nuclei. The proton and neutron densities, charge densities, mass densities were calculated by using Skyrme interactions with SI, SIII, SIV, T3, SKM and SKM* force parameters. The nuclear ground-state properties for the $^{87\text{-}102}Zr$, ^{93}Nb, ^{181}Ta isotopes are calculated. Skyrme force parameters can be found from the literature [8-12].

2 Results and Discussions

We have used the Skyrme interaction parameters for calculations with the program HAFOMN code based on a harmonic oscillator wave function (HOWF) [13]. In these calculations, the pairing equations are solved by Newton's tangential iteration. For description of the systems consisting of an odd number of particles, we have used the filling approximation. The Hartree-Fock and pairing equations are coupled, and they are solved by simultaneous iteration of the wave functions and the occupation weights [2].

In this study, we have calculated by using the Hartree-Fock method with an effective interaction with Skyrme forces parameters for the $^{87\text{-}102}$Zr, ^{93}Nb and ^{181}Ta isotopes and compared with experimental data experimental Root-Mean-Square (rms) charge density radii in Table 1.

[a] Corresponding author: halidesahan@osmaniye.edu.tr

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Experimental values were taken from Atomic Data and Nuclear Data Tables [14,15]. The nuclear charge density is a most useful observable for analyzing nuclear structure and provides information about the nuclear shape and also can be determined by clear-cut proceed [16]. It can be seen that the experimentally measured charge rms density radii little increases from ^{87}Zr (about 4.2 fm) to ^{102}Zr (about 4.5 fm) except ^{88}Zr (about 4.2 fm), ^{89}Zr (about 4.2 fm), ^{90}Zr (about 4.2 fm), ^{91}Zr (about 4.2 fm) isotopes' charge rms density radii as the mass number increases in Table 1. The experimentally measured charge rms density radii for ^{93}Nb and ^{181}Ta are about 4.3 and 5.3 fm respectively as seen in Table 1. Theoretically the calculated charge rms values are quite consistent with the theoretical calculations with all the Skyrme forces parameters. Theoretically calculated charge rms values are also quite consistent with experimental values. Especially, theoretical calculations by using the Skyrme forces parameters with SKM* is closer to experimental values. Also in Table 1, the nuclear charge rms values calculated by using Skyrme forces have been compared with the values of radius $r_o A^{1/3}$ in Liquid-Drop Model in which the number of nucleons per unit volume is roughly constant. The value of r_o has been taken as 1.25 fm from electron scattering experiments. Similar to the Hartree-Fock calculations with Skyrme forces, the radius values in Liquid-Drop Model have been little increased from 5.5 fm (for ^{87}Zr) to 5.8 fm (for ^{102}Zr) depending on the mass number A. The values of radius in Liquid-Drop Model for ^{93}Nb and ^{181}Ta are 4.3 and 5.3 fm, respectively. However theoretical calculations by using the Liquid-Drop Model are very higher than the experimental values.

We calculated mass rms radius by using the Hartree-Fock with Skyrme forces parameters for the $^{87\text{-}102}$Zr, ^{93}Nb and ^{181}Ta isotopes and we summarized the results in Table 2. For the ^{87}Zr, theoretically calculated mass rms values are quite consistent with other calculations values. The calculated neutron and proton rms radius with the Skyrme Hartree-Fock model for the same isotopes were given in Table 3 and Table 4, respectively.

The comparison of the calculated values using only the SKM* parameter charge, proton, neutron and mass densities for $^{90\text{-}94}$Zr, ^{93}Nb, ^{181}Ta isotopes are given in Fig. 1-6. For $^{90\text{-}94}$Zr isotopes at the center (r=0), the obtained values of the charge density with SKM* have approximately been increased from 0.0715 fm^{-3} (for ^{90}Zr) to 0.0717, 0.0718, 0.0719 fm^{-3} (^{91,92,94}Zr) with the increasing of the number of mass. For $^{90\text{-}94}$Zr isotopes at the center (r=0), the obtained values of the proton density with SKM* have been decreased from 0.0700 fm^{-3} to 0.0699, 0.0698, 0.0695 fm^{-3} with the increasing of the number of mass, respectively. The obtained values of the neutron density with SKM* for $^{90\text{-}94}$Zr isotopes at the center (r=0) have approximately been increased from 0.0791 fm^{-3} (for ^{90}Zr) to 0.0814, 0.828, 0.0861 fm^{-3} (^{91,92,94}Zr) with the increasing of the number of mass, respectively. The obtained values of the mass density with SKM* for $^{90\text{-}94}$Zr isotopes at the center (r=0) have approximately been increased from 0.149 fm^{-3} (for ^{90}Zr) to 0.151, 0.152, 0.155 fm^{-3} (^{91,92,94}Zr) with the increasing of the number of mass. Moreover, the obtained values of the charge and proton densities with SKM* for ^{93}Nb isotope at the center (r=0) were found to be approximately 0.717 fm^{-3} and 0.690 fm^{-3}, respectively. The obtained values of the neutron and mass densities with SKM* for ^{93}Nb isotope at the center (r=0) were also approximately 0.819 fm^{-3} and 0.151 fm^{-3}, respectively. The obtained values of the charge density with SKM* for ^{181}Ta isotope at the center (r=0) is approximately 0.597 fm^{-3}. The obtained values of the neutron, proton and mass densities with SKM* for ^{181}Ta isotope at the center (r=0) are approximately 0.585 fm^{-3}, 0.898 fm^{-3}, 0.148 fm^{-3}. In Fig. 1-4, the calculated all densities of ^{90,91,92,94}Zr isotopes are constant from about to 2 fm radius value than 5-6 fm radius value while they decreases drastically to zero after 5-6 fm for ^{90,91,92,94}Zr target nuclei. The calculated densities of ^{93}Nb are constant from about to 2 fm radius value than 5-6 fm radius value while they decreases drastically to zero after 5-6 fm for ^{93}Nb target nuclei in Fig. 5 and Fig.6. Values approximately to zero value are about in the vicinity of 7-8 fm. While the calculated densities of target nuclei $^{90\text{-}94}$Zr and ^{93}Nb at the center (at r = 0) appear to give maximum with the value near to about 2 fm radius value in Fig. 1-5. The calculated densities of target nuclei ^{181}Ta at the center appear to give maximum with the value near to about 3 fm radius value in Fig 6.

3 Conclusion

In this study, the charge, mass, proton, and neutron densities and the rms charge, mass, proton and neutron radii have been calculated for $^{87\text{-}102}Zr, ^{93}Nb, ^{181}Ta$ isotopes by using the Hartree–Fock method with an effective Skyrme force with SI, SIII, SVI, T3, SKM, SKM* and compared with experimental data. From Table 1, since the calculated theoretical charge rms values using Skyrme forces parameters are quite consistent with experimental values, we only obtained radii versus densities figures for SKM*. The radius values in Liquid-Drop Model have been little increased depending on the mass number A. These results can be contributed to understanding ground state properties for these structural fusion materials.

Table 1. The calculated rms charge density radius (in fm and r_0=1.25 fm).

	SI	SIII	SVI	T3	SKM	SKM*	$r_0A^{1/3}$	Exp [20]
^{87}Zr	4.191	4.308	4.317	4.254	4.264	4.284	5.538	4.282
^{88}Zr	4.197	4.313	4.322	4.257	4.267	4.286	5.559	4.281
^{89}Zr	4.202	4.318	4.328	4.260	4.269	4.288	5.580	4.271
^{90}Zr	4.207	4.323	4.334	4.264	4.271	4.291	5.010	4.269
^{91}Zr	4.217	4.333	4.344	4.272	4.280	4.299	5.622	4.284
^{92}Zr	4.225	4.343	4.353	4.278	4.286	4.305	5.642	4.305
^{94}Zr	4.242	4.361	4.371	4.291	4.299	4.318	5.683	4.331
^{96}Zr	4.260	4.380	4.390	4.305	4.313	4.332	5.723	4.349
^{97}Zr	4.269	4.390	4.400	4.314	4.322	4.340	5.743	4.393
^{98}Zr	4.279	4.399	4.410	4.322	4.331	4.349	5.763	4.418
^{99}Zr	4.288	4.409	4.420	4.331	4.340	4.358	5.782	4.434
^{100}Zr	4.298	4.419	4.429	4.341	4.351	4.368	5.801	4.522
^{101}Zr	4.307	4.428	4.439	4.351	4.361	4.379	5.821	4.548
^{102}Zr	4.317	4.438	4.449	4.361	4.372	4.389	5.840	4.569
^{93}Nb	4.247	4.366	4.376	4.301	4.309	4.329	5.663	4.324
^{181}Ta	5.229	5.365	5.378	5.284	5.298	5.311	7.070	5.350

Table 2. The calculated rms mass density radius (in fm)

	SI	SIII	SVI	T3	SKM	SKM*	$r_0A^{1/3}$
^{87}Zr	4.128	4.248	4.251	4.202	4.209	4.228	5.538
^{88}Zr	4.139	4.260	4.263	4.214	4.220	4.239	5.559
^{89}Zr	4.151	4.273	4.276	4.226	4.231	4.250	5.580
^{90}Zr	4.162	4.285	4.288	4.239	4.242	4.261	5.601
^{91}Zr	4.180	4.306	4.307	4.260	4.263	4.282	5.622
^{92}Zr	4.196	4.324	4.324	4.276	4.281	4.300	5.642
^{94}Zr	4.229	4.360	4.357	4.312	4.316	4.334	5.683
^{96}Zr	4.262	4.395	4.391	4.348	4.352	4.370	5.723
^{97}Zr	4.278	4.412	4.407	4.367	4.371	4.389	5.743
^{98}Zr	4.294	4.429	4.424	4.385	4.391	4.408	5.763
99Zr	4.310	4.446	4.440	4.405	4.410	4.427	5.782
100Zr	4.326	4.463	4.456	4.424	4.430	4.446	5.801
101Zr	4.341	4.479	4.472	4.443	4.449	4.465	5.821
102Zr	4.358	4.494	4.486	4.461	4.468	4.484	5.840
93Nb	4.209	4.337	4.338	4.288	4.292	4.311	5.663
181Ta	5.233	5.376	5.379	5.323	5.334	5.347	7.070

Table 3. The calculated rms neutron density radius (in fm)

	SI	**SIII**	**SVI**	**T3**	**SKM**	**SKM***	**$r_0A^{1/3}$**
^{87}Zr	4.135	4.258	4.257	4.219	4.223	4.241	5.538
^{88}Zr	4.151	4.275	4.274	4.238	4.239	4.258	5.559
^{89}Zr	4.167	4.293	4.291	4.256	4.256	4.274	5.580
^{90}Zr	4.182	4.309	4.307	4.273	4.272	4.290	5.601
^{91}Zr	4.207	4.337	4.333	4.303	4.302	4.320	5.622
^{92}Zr	4.228	4.361	4.355	4.326	4.327	4.344	5.642
^{94}Zr	4.271	4.407	4.397	4.374	4.375	4.392	5.683
^{96}Zr	4.311	4.451	4.439	4.422	4.423	4.439	5.723
^{97}Zr	4.331	4.472	4.459	4.446	4.447	4.443	5.743
^{98}Zr	4.351	4.493	4.479	4.470	4.471	4.487	5.763
99Zr	4.370	4.513	4.498	4.494	4.496	4.511	5.782
100Zr	4.389	4.533	4.517	4.518	4.520	4.535	5.801
101Zr	4.408	4.552	4.536	4.541	4.543	4.559	5.821
102Zr	4.427	4.570	4.553	4.563	4.567	4.582	5.840
93Nb	4.235	4.368	4.363	4.330	4.331	4.349	5.663
181Ta	5.270	5.420	5.413	5.386	5.395	5.408	7.070

Table 4. The calculated rms proton density radius (in fm)

	SI	**SIII**	**SVI**	**T3**	**SKM**	**SKM***	**$r_0A^{1/3}$**
^{87}Zr	4.119	4.236	4.243	4.182	4.193	4.213	5.538
^{88}Zr	4.125	4.242	4.250	4.186	4.196	4.216	5.559
^{89}Zr	4.131	4.248	4.256	4.190	4.200	4.220	5.580
^{90}Zr	4.137	4.255	4.263	4.195	4.204	4.224	5.601
^{91}Zr	4.146	4.266	4.274	4.204	4.214	4.234	5.622
^{92}Zr	4.155	4.275	4.283	4.211	4.221	4.241	5.642
^{94}Zr	4.173	4.295	4.303	4.226	4.236	4.256	5.683
^{96}Zr	4.191	4.315	4.323	4.242	4.252	4.271	5.723
^{97}Zr	4.200	4.325	4.333	4.251	4.261	4.280	5.743
^{98}Zr	4.210	4.335	4.343	4.260	4.270	4.289	5.763
99Zr	4.219	4.345	4.353	4.269	4.280	4.299	5.782
100Zr	4.229	4.355	4.363	4.279	4.291	4.309	5.801
101Zr	4.238	4.365	4.374	4.289	4.301	4.319	5.821
102Zr	4.250	4.373	4.381	4.298	4.311	4.329	5.840
93Nb	4.175	4.298	4.306	4.233	4.243	4.263	5.663
181Ta	5.179	5.312	5.328	5.230	5.243	5.256	7.070

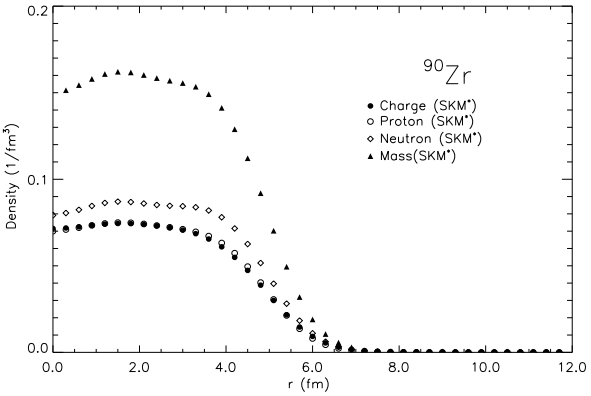

Figure 1. The calculated using the SKM* parameter charge, proton, neutron, mass densities of ^{90}Zr isotope

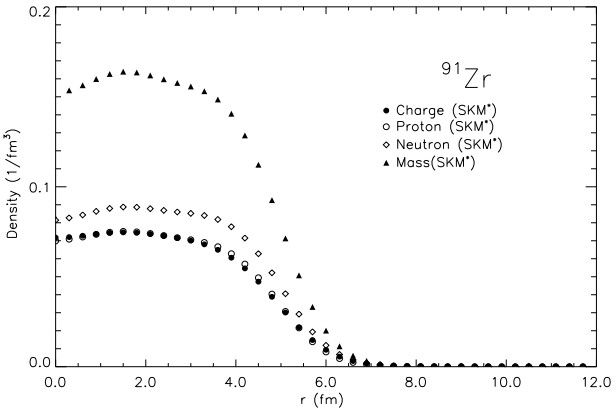

Figure 2. The calculated using the SKM* parameter charge, proton, neutron, mass densities of ^{91}Zr isotope

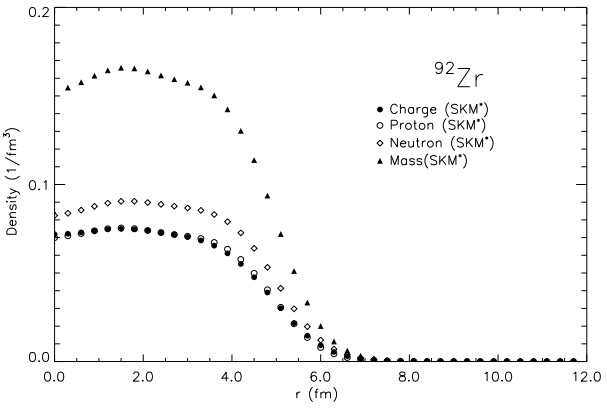

Figure 3. The calculated using the SKM* parameter charge, proton, neutron, mass densities of ^{92}Zr isotope

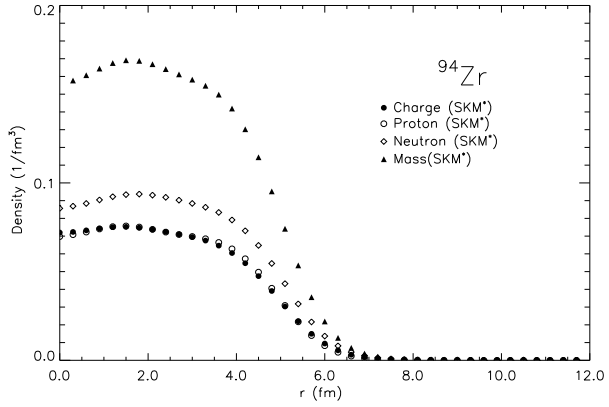

Figure 4. The calculated using the SKM* parameter charge, proton, neutron, mass densities of ^{94}Zr isotope

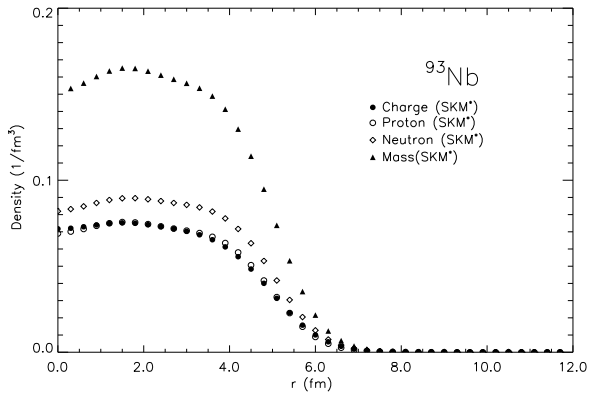

Figure 5. The calculated using the SKM* parameter charge, proton, neutron, mass densities of ^{93}Nb isotope

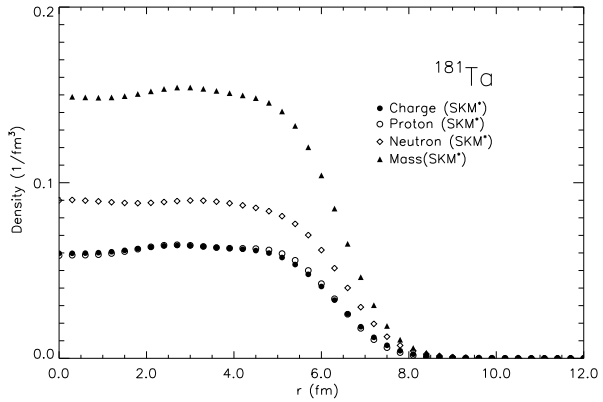

Figure 6. The calculated using the SKM* parameter charge, proton, neutron, mass densities of ^{181}Ta isotope

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