Radiation Effects in Nuclear Ceramics for the Immobilization of Radioactive Waste

A Synopsis Submitted

To

THE MAHARAJA SAYAJIRAO UNIVERSITY OF BARODA

FOR THE DEGREE OF

DOCTOR OF PHILOSOPHY

IN

PHYSICS

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1. Introduction

Nuclear energy generates a very low amount of CO_2 and other pollutants, and presently provides ~11% of the global electricity[1]. In contrast, a variety of radioactive nuclear wastes are generated at various stages of the nuclear fuel cycle (milling and mining of uranium ore, reactor operation, fuel fabrication, and used fuel reprocessing) in the nuclear power plants[1]. The ecological system safety is a major concern due to the production of radioactive nuclear waste. The adverse effect of radioactive nuclear waste on human health and the environment is a major hindrance to the widespread use of nuclear energy. Therefore, there is a necessity for safe and effective management of these hazardous and environmentally sensitive high-level radioactive wastes (HLWs)[2]. To attain this, the development of radiation-resistant materials for effective management of radioactive wastes and actinides surplus is of utmost importance. The scientific community all over the world is looking for a suitable material for the safe disposal and effective management of radioactive nuclear waste. Materials used for effective management of (involving their safe discharge and storage) radioactive wastes should be stable in radioactive environments[2]. Each material has different radiation resistance tolerance. Considering the materials for radioactive waste immobilization, the response of the material in radiation environments must be quantified for a longer period. Pyrochlore oxides have drawn a huge interest because of their remarkable chemical and physical properties[2]. The inevitable properties of the pyrochlore structural oxides such as high radiation stability, excellent thermal stability, high ionic conductivity, high thermal and chemical stability make them a suitable candidate for the potential application in hostile environments i.e., immobilization of radioactive nuclear waste and various state of the art applications such as high-temperature solid oxide fuel cells, solid electrolytes, high-temperature superconductors, photoluminescence, piezoelectricity, catalysis, thermal barrier coatings and so on[3-6].

Pyrochlore oxides, $A_2B_2X_6Y$ (where A and B are the metal cations whereas X and Y are anions) possess cubic crystal structure with the space group of $Fd\bar{3}m$[2,6]. Cations, A occupy the 16c site and cations, B occupies the 16d site; the oxygen ions, X and Y are located at the 48f and 8a positions respectively and the 8b position remains unoccupied[6].

It is noteworthy that the pyrochlore oxides crystal structure depends on the cationic radius ratio, i. e., r_A/r_B. The $A_2B_2O_7$ show pyrochlore (superlattice reflections) crystal structure with cationic radius ratio of $1.46 < r_A/r_B < 1.78$ which exhibits compositional and structural tunability of pyrochlore oxides. For the cationic radius ratio of $r_A/r_B < 1.46$, the $A_2B_2O_7$ show disordered fluorite structure[7]. The ordering/disordering of the cation and anion lattice is a distinctive feature of pyrochlore oxides structure and plays an imperative role in altering the structural, thermal, and electronic/ionic properties and radiation tolerance of the isometric pyrochlore materials[3]. Cation/anion order-disorder, defects, pyrochlore to disorder/fluorite structure transformation in the pyrochlore are correlated to its composition and external parameters, i.e., sintering temperature, applied pressure, and ion beam irradiation[7]. Chartier et al. reported that $La_2Zr_2O_7$ has a greater tendency towards cation disorder due to low formation energy (~2 eV) of cation antisite defect[8]. Owing to ease of formation of order-disorder transition, the $La_2Zr_2O_7$ should be highly resistant to radiation damage. However, the $La_2Zr_2O_7$ shows the relatively poor characteristic of radiation resistance upon ion irradiation and it became amorphized upon irradiation of 1.5 MeV Xe^+ with a dose of 5.5 dpa at room temperature[9]. Lian et al. stated that the critical amorphization dose increased with an increment in the irradiation temperatures and complete amorphization cannot be achieved above the critical temperature even at elevated ion dose because of competition between amorphization and recovery processes[9]. Kasper et al. irradiated the $La_2Zr_2O_7$ thin film using 1 MeV Zr^+ ions up to 10 displacements per atom (dpa) at room temperature and found that the simulated model exhibits the amorphization behaviour of the $La_2Zr_2O_7$ thin film[6]. In contrast, the epitaxial $La_2Zr_2O_7$ thin film upon ion irradiation revealed the polycrystalline nature up to the dose of 10 dpa[6]. Recently, the radiation stability and solubility of actinides involving $La_2Zr_2O_7$ pyrochlore have been investigated[10]. Both, the experimental and theoretical studies on the $La_2Zr_2O_7$ revealed that the incorporation of plutonium enhanced the radiation toleration characteristics of it[11].

Several studies have been performed on the viability, capability, and stability of $Gd_2Zr_2O_7$ for possible application in hostile environments. $Gd_2Zr_2O_7$ is considered a suitable and promising host candidate for radioactive waste immobilization due to its exceptional chemical and thermal stability, radiation tolerance in hostile environments, mechanical properties, and so on[2,3,5,12,13]. $Gd_2Zr_2O_7$ with $r_A/r_B = 1.46$ exhibited the order-disorder transformation instead of being amorphized upon irradiation with high energy heavy ions[14]. Wang et al. obtained the systematic improvement in the radiation tolerance with the enhancement of the Zr content in the $Gd_2(Zr_xTi_{1-x})_2O_7$ system upon ion irradiation (1 MeV Kr^{2+})[4]. $Gd_2Ti_2O_7$ system is amorphized easily at an irradiation dose of 0.2dpa. In contrast, Zn enriched pyrochlore phase (e. g., $Gd_2Zr_2O_7$) does not show evidence of amorphous phase even at an irradiation dose of 15 dpa[4]. It is worth noting that microcrystalline $Gd_2Zr_2O_7$ pyrochlore displays pyrochlore to disordered fluorite phase transformation upon irradiation (2 MeV Xe^{20+})[15]. Patel et al. reported the pyrochlore to defect fluorite phase transformation of $Gd_2Zr_2O_7$ system with enhanced electronic stopping powers (S_e) upon irradiation of swift heavy ions, i.e., 70 MeV Ni^{5+}, 90 MeV I^{7+}, and 120 MeV Au^{9+} ions[16]. Moreover, the swift xenon ions (1.43 GeV) irradiation-induced order-disorder and crystalline to amorphous phase transitions in the binary $Gd_2Zr_{2-x}Ti_xO_7$ system have been investigated by Lang et al.[17]. The Zr-enrich pyrochlore phase (e. g., $Gd_2Zr_2O_7$) favoured the order-disorder transition, i.e., the transformation from pyrochlore to defect fluorite phase structure upon irradiation. On the contrary, the Ti-enrich compositions become amorphized easily without experiencing order-disorder transformation. It is noteworthy that the radiation resistance susceptibility of pyrochlore compounds also depends on grain size along with compositions, irradiation temperature, ion fluence, structure symmetry and so on[3,12,18]. Recently, Huang et al. reported that with an increase of grain size of $Gd_2Zr_2O_7$ from 55 to 221 nm, the amorphization fraction enhances from 6.8 to 11.10 %, i.e., amorphization fraction seems size-dependent[19]. Similarly, several reports stated the nanocrystalline Au, Pd, TiNi, and spinel $MgGa_2O_4$ exhibited the enhanced radiation tolerance in comparison to their corresponding bulk counterparts[19-21]. Zhang et al. found that the nanostructured $Gd_2(Ti_{0.65}Zr_{0.35})_2O_7$ system exhibits superior radiation resistance capability in comparison to coarse-grained counterpart (>100 nm)[21]. The inverse spinel nanocrystalline $MgGa_2O_4$ (4-12 nm) tolerate the radiation doses up to 96 dpa whereas its bulk counterpart becomes amorphized even at a dose of 12 dpa[22]. It is stated that the nanocrystalline ceramics (below 100 nm) demonstrated enhanced radiation resistance than that of their bulk counterpart because of significantly higher interfacial areas and grain boundaries. The relatively more grain boundaries and interfaces act as efficient sinks for the defects produced upon radiation and facilitate the diffusion/migration of atoms, which enhances radiation resistance[23]. Moreover, the higher interfacial areas in nanostructured ceramics facilitate shorter diffusion distance for defect migration which promotes radiation resistance tolerance in the nanocrystalline ceramics[23]. On the contrary, Meldrum et al. reported that the nanocrystalline ZrO_2 (~3 nm) becomes amorphized easily upon irradiation dose of 0.9 dpa. However, bulk ZrO_2 possesses crystalline nature even irradiated with a very high dose of 680 dpa [24]. Grover et al. investigated the radiation resistance of CeO_2 microstructure upon irradiation of 100 MeV Ag ions and reported that grain size in micrometer range exhibits better radiation resistance than nanometer grain size[25]. Recently, a comparative study on the nanometer (78 nm) and micrometer (2 µm) grain size of $Gd_2Zr_2O_7$ upon irradiation (5 MeV Xe^{20+}) has been performed by Liu et al. [12]. They found that the microsized $Gd_2Zr_2O_7$ shows better radiation resistance in comparison of nanosized $Gd_2Zr_2O_7$[12]. Interestingly, Kumari et al.[18] reported that the $Gd_2Zr_2O_7$ pyrochlore phase retains the crystallinity upon irradiation of 120 MeV Au with a fluence of 1.0 x 10^{14}

ions/cm^2. However, the defect fluorite phase losses the crystallinity at the fluence of 1.0 x 10^{13} ions/cm^2, implies that the pyrochlore phase $Gd_2Zr_2O_7$ has better radiation stability rather than the defect fluorite phase. Further, they stated that along with crystal structure, the higher grain size of the pyrochlore phase could be the possible reason for better radiation resistance[18]. Recently, Liu et al. reported that the leaching rate depends on the grains size of $Gd_2Zr_2O_7$ and it is found that the leaching rate decreased with the increased grains size[3].

Here, we would like to stress that the pyrochlore compounds, $La_2Zr_2O_7$ and $Gd_2Zr_2O_7$ are suitable and promising candidates for the various state of the art applications such as high-temperature solid oxide fuel cells, solid electrolytes, high-temperature superconductors, photoluminescence, piezoelectricity, catalysis, thermal barrier coatings, and immobilization of radioactive nuclear waste. To the best of our knowledge, there is no literature available on the evaluation of the structural properties of the $La_2Zr_2O_7$ upon irradiation (1 MeV Xe^{4+} and 500 keV Kr^{2+} ions) at low (~88 K) and room temperature (300 K); and despite the several numbers of studies, the conclusive outcome of structural ordering/disordering and microsized grains of $Gd_2Zr_2O_7$ upon ion irradiation has not been investigated so far up to best of our knowledge. These results enlighten our interest towards the investigation mainly: (a) role of irradiation temperature and ion fluence on the structural modifications of $La_2Zr_2O_7$ for fundamental understanding and addressing the structure tunability for the state of the art applications, and (b) impact of structural ordering/disordering and microsized $Gd_2Zr_2O_7$ ceramics on the radiation resistance tolerance upon ion irradiation of 100 MeV iodine.

2. Objectives

The main objective of the present thesis work is to study and investigate the effect of radiation on $La_2Zr_2O_7$ and $Gd_2Zr_2O_7$ pyrochlore oxides. The structural modifications, i.e., damage/amorphization and degree of ordering/disordering in the $La_2Zr_2O_7$ upon irradiation of 1 MeV Xe^{4+} and 500 keV Kr^{2+} ions at two different temperatures, i.e., ~88 K and 300 K were investigated and discussed. Impact of structural ordering/disordering and grains size of $Gd_2Zr_2O_7$ pyrochlore on the radiation resistance engineering towards complex nuclear waste immobilization, i.e., applications for the hostile environments in the interest of safe and effective management of radioactive waste and surplus actinides were explored.

For convenience, the present thesis is divided into eight chapters and the outline of each chapter is presented herewith.

3. Classification of thesis chapters

Chapter 1: This chapter deals with the introduction and importance of pyrochlore and fluorite compounds in the application for possible use in hostile environments. The emergence of the zirconate pyrochlore for the immobilization of nuclear wastes has been described. The feasibility of a wide range of pyrochlore compounds for the immobilization of radioactive nuclear wastes has been discussed.

Chapter 2: This chapter provides detailed information about the processing techniques employed for the preparation of $La_2Zr_2O_7$ and $Gd_2Zr_2O_7$ samples. To investigate the structural modifications in the $La_2Zr_2O_7$ and $Gd_2Zr_2O_7$ upon ion irradiation, the irradiation experiments have been analyzed and explained. This chapter also describes the details of various experimental techniques which have been used for the characterization of the $La_2Zr_2O_7$ and $Gd_2Zr_2O_7$ compounds.

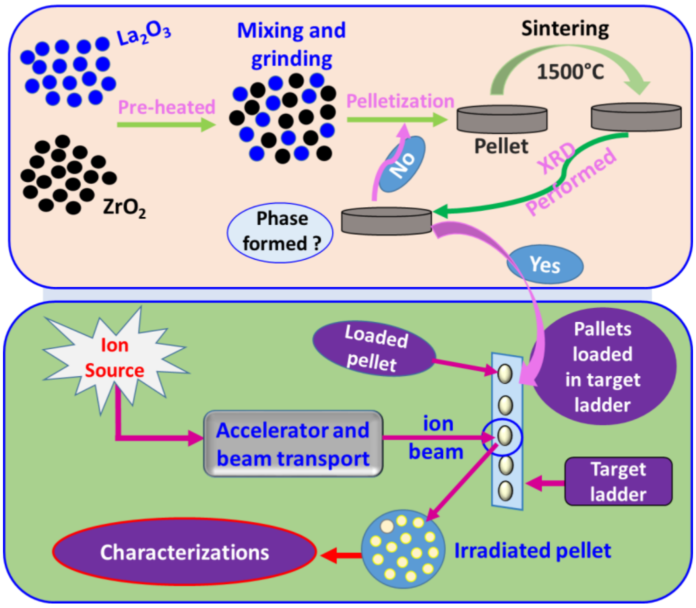

Fig. 1: Schematic shows the sample preparation and ion irradiation process.

The characterization tools that have been discussed in this chapter are namely: X-ray diffraction (XRD), grazing incidence X-ray diffraction (GIXRD), field emission scanning electron microscopy (FE-SEM), and high-resolution transmission electron microscopy (HR-TEM), and Raman spectroscopy. Each of the experimental tools has been described with their brief instrument’s part, data extraction, and analysis.

Chapter 3: This chapter deals with atomic order/disorder and grain growth kinetics of polycrystalline $La_2Zr_2O_7$, which originated due to isothermal annealing at various temperatures, i.e., 1200, 1300, and 1500°C. The prepared $La_2Zr_2O_7$ samples were examined using XRD, FE-SEM, and Raman spectroscopy. X-ray diffraction confirmed the formation of the pyrochlore phase. The impact of annealing temperature on the assessment of structural properties of $La_2Zr_2O_7$ has been discussed based on the XRD and Raman spectroscopy results. A gradual increase in the intensity of the XRD patterns as a function of annealing temperature was observed which indicates the enhancement of crystallinity. Further, Rietveld refinement of XRD patterns of $La_2Zr_2O_7$ samples exhibited that the degree of cation ordering increased with the increase of annealing temperature. Raman spectroscopy results corroborate the XRD results. The grain growth process involves densification and coarsening which favoured the formation of larger grains upon annealing at the higher temperature. FE-SEM results confirmed the evolution of grain growth with the increase of annealing temperature. The results of this investigation demonstrated that the structural modifications could be effective in designing and tailoring the pyrochlore materials for energy applications.

Chapter 4: This chapter addresses the damage/amorphization of polycrystalline $La_2Zr_2O_7$ upon ion irradiation of 1 MeV Xe^{4+} ions with a fluence of 1.0×10^{13}, 5.0×10^{13}, and 1.0×10^{14} ions/cm^2 at two different temperatures, i.e., 300 K and ~ 88 K. The pristine and irradiated $La_2Zr_2O_7$ samples were investigated using FE-SEM, GIXRD, HR-TEM, and Raman spectroscopy. The GIXRD study revealed that the degradation of the crystallinity (damage/amorphization) is significantly higher with the increase of ion fluence at ~88K in comparison to 300K. Raman spectroscopy demonstrated that the weakening and broadening of the intensity of the vibrational modes increased as a function of ion fluence at both temperatures. These results suggest that the disordering and distortion of chemical bonds are significantly prominent at higher fluence and are more pronounced at ~88 K than 300K. HRTEM results of the pristine and irradiated $La_2Zr_2O_7$ strengthen the GIXRD and Raman spectroscopy results and display that the deterioration of atomic ordering is significantly higher at ~ 88K.

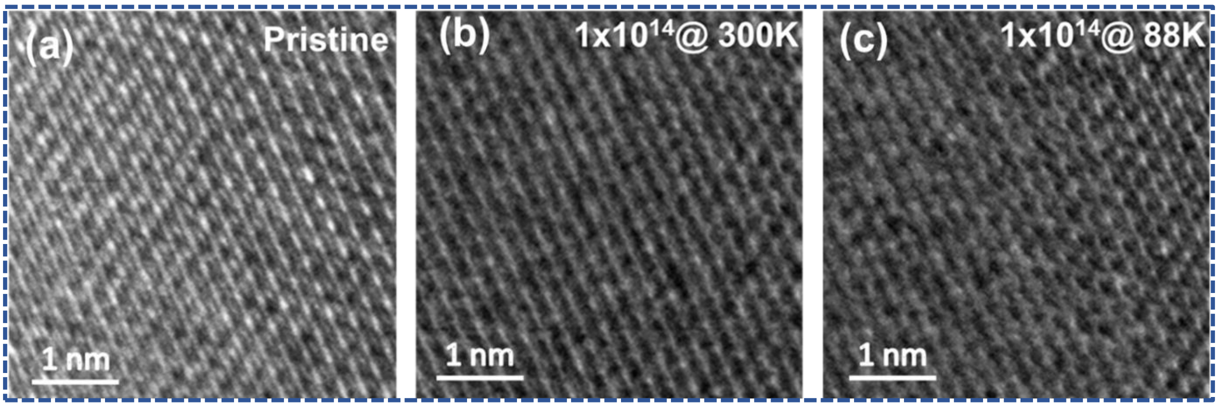

Fig. 2 HR-TEM image of pristine and irradiated $La_2Zr_2O_7$ at 300K and~ 88K with a fluence of 1.0×10^{14} ions/cm^2.

According to the earlier studies, the intrinsic and induced defects are highly immovable at low temperatures. On the other hand, the intrinsic and induced defects become highly mobile, i.e., recovery of defects on both the cation and oxygen sublattice become prominent at room temperature. Therefore, we have observed the difference in the structural modifications of the $La_2Zr_2O_7$ upon irradiation at ~88 K and 300K. These modified structural properties of the $La_2Zr_2O_7$ may be suitable for various emerging applications, such as catalysts, solid oxide fuel cells, *etc*.

Chapter 5: This chapter delineates the low energy ion irradiation-induced atomic order-disorder engineering in the $La_2Zr_2O_7$. Cation and anion disordering affect the structural and electronic properties of the isometric $A_2B_2O_7$ pyrochlore materials. The 500 keV Kr^{2+} ions irradiation-induced cation and anion ordering/disordering in the $La_2Zr_2O_7$ were investigated at 300 K and ~ 88 K. GIXRD results confirmed that the weakening and broadening of the diffraction peaks increase monotonically as a function of ion fluence at both temperatures and appear more pronounced at ~ 88 K. The cation and anion disordering seem to be ion fluence and irradiation temperature-dependent. Raman spectroscopy confirmed the deterioration of the vibrational modes with enhanced ion fluence at both temperatures and substantiated the results obtained from the GIXRD analysis. In addition, the Raman data analysis revealed the involvement of the X_{48f} oxygen in the anion disorder. The HRTEM analysis revealed that deterioration in the atomic ordering (amorphization) is significantly more pronounced at ~88 K.

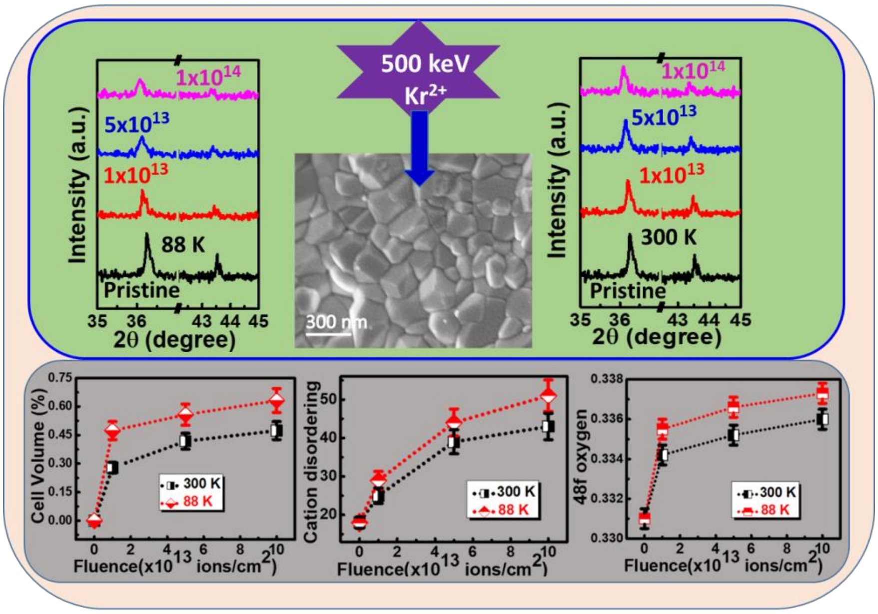

Fig. 3 Displays the structural modifications in the $La_2Zr_2O_7$ upon irradiation with 500 keV Kr^{2+} at the temperature of 300 K and ~ 88 K.

The qualitative analysis of cation and anion order/disorder and structural deformation revealed that the irradiation parameters play a crucial role in developing and altering the properties of the pyrochlore materials for technological applications.

Chapter 6: This chapter describes the impact of structural ordering on radiation resistance engineering of $Gd_2Zr_2O_7$ pyrochlore towards complex nuclear waste immobilization. The search for radiation-tolerant materials that can be utilized as hosts for the safe and effective management of radioactive waste and surplus actinides is an intense area of research in recent years. Materials for applications in hostile environments require utmost resistance to radiation damage. Owing to its complex structure, the $Gd_2Zr_2O_7$ is considered a promising candidate for the immobilization of radioactive wastes. In the present work, the different degree of order/disorder of $Gd_2Zr_2O_7$ samples were achieved easily *via* sintering at 1400°C and 1500°C. Sintering temperature-driven structural ordering/disordering and grain sizes were examined by XRD, FE-SEM, and Raman spectroscopy. To explore the effect of different degree of ordering/disordering of $Gd_2Zr_2O_7$ on radiation-induced structural modifications, the $Gd_2Zr_2O_7$ samples were irradiated with 100 MeV I^{7+} at the fluence of 1×10^{14} ions/cm^2.

The irradiation-induced structural modifications seem to be structural order/disorder dependent. Both the XRD and Raman spectroscopy results demonstrate that the highly ordered pyrochlore phase of $Gd_2Zr_2O_7$ possesses superior radiation resistance tolerance as compared to the corresponding disordered pyrochlore $Gd_2Zr_2O_7$. Analysis of the results shows that the ordered pyrochlore phase $Gd_2Zr_2O_7$ is transformed into disordered pyrochlore. Assessment of radiation resistance of GZO samples establishes the feasibility of it for the possible applications in hostile environments such as radiation tolerant hosts for safe and effective management of radioactive nuclear waste and surplus actinides.

Chapter 7: This chapter elucidates the electronic excitation induced pyrochlore to defect fluorite phase engineering of $Gd_2Zr_2O_7$ pyrochlore for feasible immobilization of nuclear waste. The materials with complex structures with a tendency to accommodate lattice disorder have been considered suitable for extremely high resistance to radiation damage. The pyrochlore phase $Gd_2Zr_2O_7$ was fabricated *via* a simple and economical solid-state process. The pyrochlore-defect fluorite phase engineering of $Gd_2Zr_2O_7$ has been investigated upon irradiation of 100 MeV I^{7+} ions at various fluences, i.e., 1.0×10^{12}, 3.0×10^{12}, 1.0×10^{13}, 3.0×10^{13}, and 1.0×10^{14} ions/cm^2. The pristine and irradiated $Gd_2Zr_2O_7$ samples were examined using FE-SEM, XRD, and Raman spectroscopy. X-ray diffraction study shows the electronic excitation-induced phase transformation from ordered pyrochlore to defect fluorite phase structure upon ion irradiation. The qualitative analysis of the Raman spectra of $Gd_2Zr_2O_7$ samples demonstrated the order-disorder phenomenon upon irradiation of 100 MeV iodine ion with the increase of fluence from 1.0×10^{12} to 1.0×10^{14} ions/cm^2. Both the XRD and Raman spectroscopy results quantify the disorder engineering without experiencing an amorphization process upon high electronic excitation. The phase engineering (pyrochlore to defect fluorite phase) instead of being amorphized demonstrates the capability of the present $Gd_2Zr_2O_7$ samples for feasible immobilization of nuclear waste.

Chapter 8: This chapter summarizes the overall concluding remarks drawn from the thesis. This chapter also highlights the feasible scope of outspreading this work in the near future.

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List of Publications:

I. Peer-reviewed journals: From thesis work

1. <u>Asha Panghal</u>, K. Kulriya, Y. Kumar, F. Singh, and N. L. Singh, Investigations of atomic disorder and grain growth kinetics in polycrystalline $La_2Zr_2O_7$,

Appl. Phys. A 125 (2019) 428. **Impact Factor-1.810**

2. **<u>Asha Panghal</u>**, Y. Kumar, P. K. Kulriya, P. M. Shirage, N. L. Singh, Structural assessment and irradiation response of $La_2Zr_2O_7$ pyrochlore: Impact of irradiation temperature and ion fluence, ***J. Alloys Compd.*** 862 (2021) 158556. **Impact Factor-4.650**

3. **<u>Asha Panghal</u>**, Y. Kumar, P.K. Kulriya, P.M. Shirage, N.L. Singh, Atomic order-disorder engineering in the $La_2Zr_2O_7$ pyrochlore under low energy ion, ***Accepted***, ***Ceramics International,*** Manuscript ID: CERI-D-20-13556R1. **Impact Factor-3.830**

4. **<u>Asha Panghal</u>**, Y. Kumar, N.L. Singh, Radiation resistance engineering of $Gd_2Zr_2O_7$ pyrochlore towards complex nuclear waste immobilization: the role of structural ordering and grain size, *J. Alloys Compd., Under Review*.

5. **<u>Asha Panghal</u>**, Y. Kumar, N.L. Singh, Exploring the radiation resistance tolerance of $Gd_2Zr_2O_7$ pyrochlore for application in hostile environments, *Under Preparation.*

*II.*International and National Conferences/Schools/Workshops:

(a) International:

1. <u>Asha Panghal</u>, N. L. Singh, School on Accelerator Science and Technology, 16th May- 27th May **2016**, Inter-University Accelerator Centre, New Delhi, India.

2. **<u>Asha Panghal</u>**, N. L. Singh, School on characterizations of materials, 04-09th September **2017**, Inter-University Accelerator Centre, New Delhi, India.

3. <u>Asha Panghal</u> and N. L. Singh, International Conference on High Energy Radiation and Applications, 10th-13th October **2017**, The M. S. University of Baroda, Vadodara, Gujarat, India

4. <u>Asha Panghal</u>, N. L. Singh, Joint ICTP-IAEA Workshop on Fundamentals of Vitrification and Vitreous Materials for Nuclear Waste Immobilization, 06-10th November **2017,** *International Centre for Theoretical Physics***, Trieste, Italy** (***Oral presentation***).

5. <u>Asha Panghal</u>, N. L. Singh, Joint ICTP-IAEA International School on Nuclear Waste Actinide Immobilization" 10-14th September **2018**, *International Centre for Theoretical Physics, UNESCO****, Italy*** (***Oral presentation***).

6. <u>Asha Panghal</u> and N. L Singh, 5th International Conference on "Ion beams in materials engineering and characterization**"** (***IBMEC***) 9-12th October **2018**, IUAC, New Delhi, India ***(Best Poster Award_1st prize)***

7. <u>Asha Panghal</u> and N. L Singh, Indo-French conference on "Radiation damage in Nuclear Materials" 18-20th February **2019**, held at Amity University Noida and IUAC New Delhi, India.

8. **<u>Asha Panghal</u>**, N. L. Singh, Joint ICTP-IAEA International School on Radioactive Waste Cementation, 16th Oct-25th Nov **2020,** *International Centre for Theoretical Physics,* ***Trieste, Italy.*** *(Virtual School_Oral presentation).*

9. **<u>Asha Panghal</u>,** N. L Singh, International conference (online) on Ion Beams in Materials Engineering and Characterization (***IBMEC-2020***), 8-11th, December **2020**, held at IUAC Delhi, India (*Online mode*).

(b) National:

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