



Article Atomic Insights into the Structural Properties and Displacement Cascades in Ytterbium Titanate Pyrochlore (Yb₂Ti₂O₇) and High-Entropy Pyrochlores

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Abstract: Pyrochlore oxides $(A_2B_2O_7)$ are potential nuclear waste substrate materials due to their superior radiation resistance properties. We performed molecular dynamics simulations to study the structural properties and displacement cascades in ytterbium titanate pyrochlore $(Yb_2Ti_2O_7)$ and high-entropy alloys (HEPy), e.g., YbYTiZrO₇, YbGdTiZrO₇, and Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO₇. We computed lattice constants (LC) (a₀) and threshold displacement energy (E_d). Furthermore, the calculation for a₀ and ionic radius (r_{ionic}) were performed by substituting a combination of cations at the A and B sites of the original pyrochlore structure. Our simulation results have demonstrated that the lattice constant is proportional to the ionic radius, i.e., a₀ α r_{ionic}. Moreover, the effect of displacement cascades of recoils of energies 1 keV, 2 keV, 5 keV, and 10 keV in different crystallographic directions ([100], [110], [111]) was studied. The number of defects is found to be proportional to the energy of incident primary knock-on atoms (PKA). Additionally, the E_d of pyrochlore exhibits anisotropy. We also observed that HEPy has a larger E_d as compared with Yb₂Ti₂O₇. This establishes that Yb₂Ti₂O₇ has characteristics of lower radiation damage resistance than HEPy. Our displacement cascade simulation result proposes that HEPy alloys have more tendency for trapping defects. This work will provide atomic insights into developing substrate materials for nuclear waste applications.

Keywords: molecular dynamics simulation; ytterbium pyrochlore oxides; nuclear waste substrate; displacement cascades; lattice constants; high-entropy alloys; LAMMPS

1. Introduction

Despite the environment-friendly and high-efficacy energy source, nuclear energy has a few distinctive concerns [1]. Commercial use of nuclear power is only evident when radioactive waste management is done under a proper strategy. Therefore, the reprocessing of spent fuel is an important part of ensuring nuclear safety and environmental safety. Nuclear wastes have different forms depending on the sources and radioactive concentration [2]. Solidification of liquid waste is a common process for managing nuclear waste disposal. In this regard, the most common processes are vitrification and synroc methods [3]. Although borosilicate glass is being used frequently as a nuclear waste substrate matrix, having low solubility of actinide elements restricts their usage [4]. An alternate substitute to solve this limitation is pyrochlore ceramics due to their superior durability, and better potential at high temperatures and humid environments [5,6]. Moreover, ceramics have high values of waste loading as compared to glass [7]. The ceramic-based substrate with the minor addition of an ionic concentration has higher radiation stability and excellent chemical and physical properties [8]. Long-term radiation damage is critical for a nuclear waste disposal strategy [9]. Pyrochlore has been developed rapidly as high-entropy ceramics waste substrate materials in recent years [10,11]. Future state-of-the-art nuclear reactors involve the



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Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). recycling of nuclear fuels, burning of minor actinide series, and decontamination of fission fragments [12]. Ytterbium titanate pyrochlores (Yb₂Ti₂O₇) have been demonstrated to be an effective waste substrate material for pyrochemical reactions [13,14]. They are used as waste forms for immobilizing radioactive waste, particularly high-level radioactive waste (HLW) [13,14]. It is also notable that the aforementioned pyrochlore serves as a surrogate for actinides like plutonium and americium. Thus, making it a suitable compound for studying waste immobilization behaviors. Moreover, ytterbium titanate pyrochlores have inherent radiation resistance due to their open crystal structure, which allows them to accommodate radiation-induced defects [15].

Minervini et al. reported disorder in different pyrochlore oxides using the atomic-scale simulation method. Additionally, pyrochlore demonstrated stability range dependence on the relative size of cations [16]. Brendan et al. have investigated the relationship between the structural and bonding energy in lanthanide pyrochlore oxides (Sn_2O_7) and found that the position parameter of the oxygen vacancies is inversely proportional to the lattice parameter. Recently, Zhang et al. have reported on the machine learning (ML) methods to determine lattice constants of different multi-substitutional pyrochlores in the range of 9–11 Å [17]. Moreover, the pyrochlore stannate ($Ce_2Sn_2O_7$) demonstrated a temperature-dependent anisotropic nature [18]. Superconductivity of ternary pyrochlore oxide $(Cd_2Re_2O_7)$ was reported by Sakai et al., at 1.1 K, and the lattice constant was found to be 10.22 A at room temperature [19]. Liyuan et al. performed molecular dynamics to study structural and elastic properties of different pyrochlores under numerous combinations of A and B cations. It was found that displacement energy in pyrochlores strongly depends on the energy of the incident PKA's as well as their atomic masses [20]. They also reported that lattice parameters and the atomic radius predominantly affect structural as well as thermal properties. Chartier et al. performed molecular dynamics simulations to study displacement cascades in lanthanum zirconate pyrochlore (Ln₂Zr₂O₇) with uranium ions bombarded with 6 keV at 350 K along different orientations. It was observed that the model does not lose its crystallinity [21]. It is further reported that the displacement cascades are determinants of material radiation stability at elevated temperatures [22]. Atomicscale radiation damage studies in pyrochlores ($Gd_2Zr_2O_7$) have demonstrated healing mechanism during radiation [9,23]. Moreover, a combination of different anions and cations results in a radiation-resistant response of pyrochlores [24]. Pyrochlores have disordered structures due to irradiation and alteration of thermodynamics [25]. Pyrochlores are known for their radiation-tolerant behavior primarily because of their inherent structural stability. Their structure allows migration and annihilation of defects, minimizing their impact on the material's overall properties.

High-entropy pyrochlores refer to a class of materials that exhibit high configurational entropy due to the random distribution of multiple cations on the crystal lattice sites. These materials have been studied for various applications, including radiation tolerance. High-entropy pyrochlore (HEPy) oxides synthesized with Yb₂Ti₂O₇ are obtained by substituting the cations in the pyrochlore structure and they have displayed higher radiation resistance than individual pyrochlores [26–29]. Atomic-scale simulation results have also displayed that radiation resistance is affected by the addition of Zr content in HEPy [30]. Defect dynamics in pyrochlore-type structures are quite difficult to determine in experimental studies due to their complex structure and irradiation-associated phenomena [9,20]. The displacement cascades involve the initiation of damage in the materials alternately determine the long-term possible outcomes. Atomic-scale simulation methods can shed light on determining the fundamental material properties and interaction mechanisms in pyrochlores [24,31] It is also important to mention that a limited number of experimental and simulation studies have been performed on the behavior of different pyrochlores under radiation [9,26,32–34]. Molecular dynamics simulations have been applied to study the influence of displacement cascades on the microstructural properties of different pyrochlores [9,32]. Computer simulations interpret the radiation damage as a predictive tool for processing the experiments. The simulation models describe the physics behind the

phenomena responsible for the radiation damage mechanism in irradiated material by providing valuable tools observed in nuclear power plants (NPP). Numerous radiation damage studies have been reported on metals and alloys [35–41]. This study will serve as a predictive model for providing insight into expected behavior in radioactive environments.

This article studies three aspects of pyrochlore oxides. Primarily, interatomic potential was established by parametrizing existing literature and later validated through calculation for LC, r_{ionic} , and E_d of different combinations of A and B in pyrochlore structures. Furthermore, displacement damage cascade simulations in Yb₂Ti₂O₇ were performed with each constituent element. The primary knock-on atom's energies (E_{PKA} ~1, 2, 5, and 10 keV) with different incident directions were used for studying the effect of energy dependence. Moreover, displacement cascades keeping the same energy were studied for HEPy to determine its radiation resistance as compared to Yb₂Ti₂O₇.

2. Computational Details and Methodology

2.1. Crystal Structures

Pyrochlores have cubic fluorite-type structures containing 5 or more elements with oxygen-deficient vacancies having A₂B₂O₇ type structure with A (rare-earth) and B (transition metal) being different cations [42,43]. The 'A' position coordinated with 3⁺ cation atoms while the 'B' position coordinated with 4⁺ cation atoms, e.g., 3⁺ cations (La³⁺, Nd³⁺, Gd³⁺, Sm^{3+} , and Y^{3+}) and 4^+ cations (Zr^{4+} , Ti^{4+} , and Mo^{4+}) [44]. Moreover, 1/8 of the oxygen atoms are vacant to balance the charges [5]. The different ion combinations are used to compute different structural properties. The crystal structure is developed by Visualization of Electronic and Structural Analysis (VESTA) [45]. The lattice parameter for pyrochlore oxide was set as 10.194 Å. The initial model comprised eight unit cells with 88 atoms per unit cell with the Fd3m group having composition Yb₁₆Ti₁₆O₅₆ with a unit cell of volume 1059.578190 A³. Periodic boundary conditions were applied along axes. The initial structure was equilibrated using the steep decent method (SD) since this method is considered a quick approach for an optimal efficient solution [46]. For HEPy modeling, the selection of compound $Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO_7$ represented in equivalent to original $Yb_2Ti_2O_7$ structure with a stoichiometric ratio replacing Yb₂ \rightarrow Yb Yb \rightarrow (Yb_{0.5}Y_{0.5}) (Eu_{0.5}Gd_{0.5}) and Ti₂ \rightarrow Ti $Ti \rightarrow Ti Zr$. In other words, we can understand it by considering that the atomic number ratio at the A-site is doped with three elements Y, Eu, and Gd with a total of four elements while the B-site is doped with two elements Ti and Zr with a total of three elements. The element in atomic proportion is represented as Yb:Y:Eu:Gd:Ti:Zr \rightarrow 1:1:1:1:2:2 resulting in the formation of $Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}Ti ZrO_7$. Figure 1 displays the computational models of unit cells of all models, where (a) is an MD snapshot of a relaxed computational model under study and (b) is a unit cell of a generic representation of pyrochlore [47], and (c-f) represent unit cells of Yb₁₆Ti₁₆O₅₆, YbYTiZrO₇, YbGdTiZrO₇, and Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO₇, respectively. The composition of each pyrochlore is mentioned as labelled in Figure 1.

The characteristic crystal structure of pyrochlores consists of a network of cornersharing tetrahedra, which provides an open framework that can accommodate defects induced by radiation damage [48,49]. Molecular dynamics simulations were performed by a large-scale atomic/molecular massively parallel simulator (LAMMPS) developed by Plimpton [50] and structure analysis and visualization were done by OVITO [51].





Figure 1. Schematic representation of the computational model and a unit cell of pyrochlore, (a) Snapshot of a computational unit cell model, $Yb_{16}Ti_{16}O_{56}$, (b) Generic representation of a unit cell of pyrochlore $A_2B_2O_7$ where A and B are transition metals [43], (c) labeled structure of $Yb_{16}Ti_{16}O_{56}$, (d) $Yb_8Y_8Ti_8Zr_8O_{56}$, (e) $Yb_8Gd_8Zr_8Ti_8O_{56}$, and (f) $Yb_4Y_4Gd_4Eu_4Zr_8Ti_8O_{56}$ equivalent of $Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}ZrTiO_7$. The subscript indicates the number of particular elements in the unit cell.

2.2. Interatomic Potential

In MD simulation, realistic interatomic potentials are very crucial for reliable results [52]. The interatomic potential was modified by a coupling potential developed in earlier studies [24,53]. This potential was tested for replicating equilibrium lattice constants and lattice constants reported in earlier studies [54,55]. The potential function is divided into two parts and all pair interactions are described separately. The short-range combination of ZBL (Ziegler-Biersack-Littmark) potential and Buckingham potential are adjoined with a fitting function for smooth truncation. The long-range Coulomb potential is described by particle–particle–particle–mesh solver (PPPM) summation algorithm having accuracy up to 10^{-4} and cutoff radius ($r_{cutoff} = 10$ Å) [56]. The Buckingham potential results in negative infinity due to short-range interactions whereas ZBL potential is more realistic for charged modes at short-range interactions [57]. The piecewise interatomic potential of Yb₂Ti₂O₇ is expressed in Equation (1), where $r_{1,2}$ is the active range of potentials. The ZBL potential and Buckingham potential are fitted with a fourth-order exponential spline function represented as $V_{spline fun.}(r_{ij}) = exp (c_1 + c_2r_{ij} + c_3r_{ij}^2 + c_4r_{ij}^3)$ for smooth interconnection, where c_{1-4} are spline constants.

$$V(r_{ij}) = \begin{cases} V_{ZBL}(r_{ij}) & r_{ij} < r_{1} \\ V_{spline \ fun.}(r_{ij}) & r_{1} < r_{ij} < r_{2} \\ V_{Buck.}(r_{ij}) & r_{2} < r_{ij} < r_{ij} \\ 0 & r_{cut} < r_{ij} \end{cases}$$
(1)

The ZBL potential is defined as $V_{ZBL} = \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2 e^2}{r_{ij}} G(\alpha)$, where $G(\alpha) = 0.18118e^{-32\alpha} + 0.5099e^{-0.9423\alpha} + 0.2802e^{-0.4029\alpha} + 0.02817e^{-0.2016\alpha}$ and $\alpha = \frac{r_{ij}(Z_1^{0.23}+Z_2^{0.23})}{0.8854a_0}$. Regarding the notation in the above expression, ϵ_0 represents dielectric constant, a_0 represents Bohr's radius, e is the electronic charge, and Z_1 , Z_2 are the atomic number of elements. The atomic numbers of Yb₇₀, O₈, and Ti₄₈. The potential function of Buckingham $V_{Buck.}(r_{ij})$ potential is represented as a function of distance in Equation (2), where A_{ij} , ρ , and C_{xy} are element-dependent potential parameters.

$$V_{Buck.}(r_{ij}) = A_{ij} e^{-\frac{r_{ij}}{\rho}} - \frac{C_{xy}}{r_{ij}^{6}}$$
(2)

The Buckingham potential function for Yb and O satisfy conditions in Equation (2). The values of the parameters are set for each computed pair in Table 1 as reported by earlier studies [20,53]. For Ti–O, the value of C_{xy} is adjusted for smooth truncation. Before testing the potential further, interatomic potentials were coupled through a splined function to ZBL repulsive and Buckingham functions. The resulting functions are plotted in Figure 2. The connected potentials for cation–anion/anion–anion are computed through Table 1, while cation–cations are defined by pair style automatically computed by LAMMPS as mentioned in the previous studies [58,59].

Table 1. Buckingham potential and splined function parameters [20,53].

Pair (s)	A _{ij} (eV)	ρ (Å)	C _{xy} (eVÅ ⁶)	c_1 (e V Å $^{-1}$)	$c_2 (eV \text{\AA}^{-2})$	$c_3 (eV \text{\AA}^{-3})$	c_4 (eVÅ ⁻⁴)	r_1 (Å)	r ₂ (Å)
Yb-O	1649.80	0.3386	16.57	10.40	-8.38	3.08	-0.55	0.6	1.3
Ti-O	2131.40	0.3038	0.400	10.62	-14.80	-14.74	-6.28	0.3	2.0
0-0	9547.96	0.2192	32.00	9.355	-10.71	6.23	-1.68	0.8	2.1



Figure 2. Potential energy (V_{ij}) as a function of distance (r_{ij}) between pairs fitted by splined ZBL and Buckingham for (**a**) Yb-O, (**b**) O-O, and (**c**) Ti-O.

2.3. Displacement Cascades Simulations

Displacement cascade simulations for all cases were performed through molecular dynamics code LAMMPS [60]. A system having dimensions $10 \times 10 \times 10$ with a total of 88,000 were constructed. Our calculation for lattice parameters resulted in 10.09 Å with periodic boundary set along all axes. The interatomic-potential function was employed as mentioned in the previous section. After completing the preliminary settings, thermal relaxation was performed initially using a canonical (NVT) ensemble at 300 K at a timestep of 0.001 ps. After the thermal relaxation, the model was relaxed again using a microcanonical ensemble (NVE) at a time step of 0.0001 ps to ensure the system had attained sufficient equilibrium before proceeding with the displacement cascades simulation. For damage cascade simulations, the recoil energies were chosen as 1 keV, 2 keV, 5 keV, and 10 keV. The selected PKA's Yb atom and the PKA's angles are along the positive Z axis. The direction of PKA was set at 45° along the xy plane at 7° to avoid channeling effects.

3. Results and Discussion

3.1. Calculation for Equilibrium Lattice Constant and Ionic Radii

The sites on A and B in the pyrochlore structure have different ions and their combination affects the properties of the pyrochlores. An important parameter of the unit cell is the lattice constant and its equilibrium properties. Figure 3 displays total energy as a function of the LC of Yb₂Ti₂O₇. The concave curve indicates that the energy of the system will reach the minimum at a certain equilibrium lattice constant. The curve fitting is obtained by a polynomial function. The equilibrium lattice constant was found to be 10.05 Å which agrees with the results reported earlier [47,53].



Figure 3. Relationship between system energy as a function of LC in Yb₂Ti₂O₇.

We tested changing different cations at the A site, i.e., Lu³⁺, Yb³⁺, Er³⁺, Y³⁺, Gd³⁺, Eu³⁺, Sm³⁺, Nd³⁺, La³⁺, and Ce³⁺ while the cation at the B site was Ti⁴⁺, e.g., the first

entry in Table 2 is represented as $Lu_2Ti_2O_7$. The equilibrium lattice constant (LC) and ionic radius (r_{ionic}) were calculated for both combinations and compared with the existing literature. Table 2 represents the calculation for the LC and r_{ionic} of different ions at site A. The calculations indicate that LC is caused by the replacement of ions proportional to r_{ionic} . Our calculations are in good agreement with other studies [18,61–64]. The preliminary fitting leads to the desired value and replicates the validity of the potential for further testing the displacement cascades of models.

a_o (Å) Ion (s) r_{ionic} (Å) Lu³⁺ 0.977, 0.861 [18], 1.032 [62] 9.988, 10.291 [18], 10.011 [61] Yb³⁺ 0.985, 0.87 [18], 1.042 [62] 10.007, 10.34 [18], 10.03 [63] Er³⁺ 10.055, 10.35 [18], 10.069 [63] 1.004, 0.89 [18], 1.004 [62] Y³⁺ 10.056, 10.37 [18], 10.080 [61] 1.019, 0.90 [18] Gd^{3+} 1.053, 1.107 [61] 10.136, 8.34 [61], 10.171 [61] Eu³⁺ 1.066, 1.120 [62] 10.159, 10.192 [63] Sm^{3+} 1.062, 1.079 [62] 10.184, 10.211 [63] Nd³⁺ 1.109, 0.98 [18], 1.163 [62] 10.231, 10.56 [18] Ce³⁺ 1.143, 1.196 [62], 1.14 [63] 10.343, 10.65 [18], 10.6 [63] La³⁺ 1.164, 1.03 [18], 1.16 [64] 10.324, 10.7026 [18]

Table 2. Calculation for LC and r_{ionic} by changing A-site cations while keeping B site as Ti⁴⁺.

Figure 4 displays the XRD pattern of Yb₂Ti₂O₇, YbYTiZrO₇, YbGdTiZrO₇, and Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO₇. The peaks of HEPy exhibit the characteristics of original cubic pyrochlores with Fd-3m and an LC of 10.19478 Å, 10.19497 Å, 10.19504 Å, 10.19513 Å were found for simulated structures. X-ray dispersion coefficients for $\lambda = 1.54059$ Å with CuK α were chosen during the XRD pattern. The obtained values are in good agreement with other studies on pyrochlores [65,66].



Figure 4. XRD pattern of Yb₂Ti₂O₇, YbYTiZrO₇, YbGdTiZrO₇, and Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO₇.

3.2. Threshold Displacement Energy (E_d)

The incident energy of primary knock-on atoms (E_{PKA}) exceeds the constraints of the entire force field and leaves a vacancy. This minimum energy (E_{min}) required to displace

an atom from its lattice site is known as threshold displacement energy (E_d) [32]. The theoretical calculations displayed that off-site threshold energy depends on crystallographic direction, temperature, orientation of incident PKA, energy, and type of incident particles.

We have computed the threshold energy of Yb₂Ti₂O₇ initially by selecting Yb and Ti with O atoms as incident PKA along [100], [110], and [111] axes. The E_d is displayed along the orientation in Figure 5. It can be seen that $E_{d (Ti)} >> E_{d (Yb)} > E_{d (O)}$. We have seen that E_{d} is anisotropic. Our findings are in agreement with other studies [67,68].



Figure 5. E_d as a function of incident PKA for Yb₂Ti₂O₇ along with bombardment directions.

The calculation of the threshold energy (E_d) of high-entropy pyrochlore YbYTiZrO₇ was formed by doping the Y element at the A site and the Zr element at the B site. The atomic number ratio for simulated pyrochlore with substitution is set as Yb:Y:Ti:Zr \rightarrow 1:1:11. Later, A-site is doped with three elements as Y, Eu, and Gd while B-site is doped with a total of four elements in equal atomic proportion of seven constituent elements, i.e., Yb:Y:Gd:Eu:Ti:Zr \rightarrow 1:1:11:2:2 resulting in the formation of Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO₇. Table 3 compares the average E_d of two simulated models with incident PKA's directions. It is established that E_d(Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO₇) > E_d(Yb₂Ti₂O₇). This establishes that HEPy is less prone to defects [67]. The values of Yb are not much different from the results in Figure 4, but the value of Ti is 2 to 4 times higher, and the Ed value of O is 10, 50, or more times that of Yb₂Ti₂O₇. This difference is due to the fact that high-entropy alloys have a more complex structure. This complexity can lead to higher E_d due to strong bonding, defects, and strains [43,47,69,70].

Table 3. E_d as a function of different incident PKA's in HEPy models.

Types of PKA	PKA Direction	E _d (eV)	Types of PKA	PKA Direction	E _d (eV)
	[100]	60	Ti	[100]	1182
Yb	[110]	60		[110]	1177
	[111]	66		[111]	625
	[100]	146	Zr	[100]	430
Y	[110]	146		[110]	431
	[111]	174		[111]	426
	[100]	93		[100]	1769
Gd	[110]	93	0	[110]	1521
	[111]	84		[111]	343
	[100]	85			
Eu	[110]	85			
	[111]	128			

3.3. Effect of Displacement Cascades on Energy and Direction of PKA

Irradiated materials are associated with displacement cascades. The displacement cascades are divided into different subcascades during bombardment of incident neutrons and ion implantation. The displacement cascades with different incident PKA's are represented in Figure 6.



Figure 6. Number of defects ($N_{defects}$) as a function of time under different energy PKA damage of Yb₂Ti₂O₇ bombarded with Yb ions of different energies.

As the energy of the initial PKA increases, the total number of defects of various atoms increases due to an increase in the mean free path between atoms. Higher E_{PKA} produces larger area cascades which have a higher possibility of reaching E_d [32]. The total number of defects will have a characteristic of rapid growth and then annihilate with time. This situation is generally referred to as defect recombination and permanent defect after radiation. In Figure 7, it can be noted that during the initial stage of the simulation cascade, collision initiated a rapid accumulation of defects which occurred in the pyrochlore lattice. The number of defects reached a peak at 0.3 ps and afterwards the size of the cascade continuously reduced. The defects stabilized at 0.9 ps leaving permanent defects.



Figure 7. Displacement cascades in $Yb_2Ti_2O_7$ bombarded with 5 keV Yb at different timesteps. Blue colors are vacancies whereas purple is interstitials.

During the cascade simulations, incident PKA was located at the lower left corner and moved along the diagonal. The effect of incident direction is investigated with Yb incident with 5 keV along the *X*-axis inclined at 45° at an interval of 5° with a 7° channeling angle along the *Z*-axis. The relation between incident angle as a function of time is expressed in Figure 8. It can be seen that smaller inclination angles have a lower number of defects. This is due to the fact that higher inclination angles are associated with lower threshold energies of incident PKA's as well as successive overlapping cascades [32].



Figure 8. Number of surviving defects as a function of (**a**) Time and (**b**) inclination angle of incident 5 keV Yb in Yb₂Ti₂O₇.

To observe the effect of ions on inclination angle, we compared the effect of defect evolution at lower and higher inclination angles by a 5 keV Yb atom. It is also known from Table 3 that Ti has higher values of E_d as compared to other constituents. The relation between the number of defects as a function of time is displayed in Figure 9 for the different incident directions of PKA. It is seen that Ti atoms and Yb atoms are almost the same in 55° (Figure 9a) whereas Yb is double in Figure 9b. In both cases, O has a higher number of defects than other constituents and a higher angle has twice the number of defects. Therefore, it is more difficult to produce more defects in 55° inclination under the same energy of incident PKA.



Figure 9. The number of defects of different types of atoms at an inclination of (a) 55° and (b) 85°.

3.4. Displacement Cascades in HEPy

This effect of displacement cascades on HEPy is studied by doping different elements on A and B sites of the pyrochlore $Yb_2Ti_2O_7$ structure. We have selected Zr at B sites while the A site is changed forming three kinds of HEPy, i.e., YbYTiZrO₇, YbGdTiZrO₇, and Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO₇. The displacement cascades formed by Yb with 5keV and defects morphology in HEPy are compared with Yb₂Ti₂O₇. The comparison is based on the analysis and defect morphology. Figure 10 displays the displacement cascade at its peak and after defect annihilation with Yb incident PKA of 5 keV. The defect forms of $Yb_2Ti_2O_7$ and the other three high-entropy pyrochlores are compared. The subscript for each displays the peak defects N_{max} and after annihilation. It is noted that the area of displacement cascades is larger for $Yb_2Ti_2O_7$ whereas the number of defects formed by displacement cascades in HEPy is higher than pyrochlore whereas $Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO_7$ has a lower number of surviving defects. For all the models, the direction of PKA coincides with the defects cluster direction. We have reason to believe that high-entropy pyrochlore has a better radiation resistance compared with $Yb_2Ti_2O_7$. It is also seen from the displacement cascade snapshots the characteristic of limiting the circumferential development of defects and reducing the damage volume in HEPy.



Figure 10. Evolution of Displacement cascades in $Yb_2Ti_2O_7$ YbYTiZrO₇, YbGdTiZrO₇, and $Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO_7$ at timesteps 0.3 ps and 0.9 ps. The number of surviving defects considerably reduced with the increase of alloying constituent.

Higher energy incident PKA are reported to have a higher number of surviving defects [14,71,72]. The number of defects as a function of time are compared for HEPy and pyrochlore as is plotted in Figure 11. It can be seen from Figure 10 that the number of defects corresponding to YGdEu doped HEPy is lesser in all cases. The surviving defects in undoped pyrochlore are relatively larger than doped ones. The defect growth rate, defect disappearance rate, and defect number annihilation is faster in HEPy, especially Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO₇. It is preliminarily due to the fact that HEPy provides a large number of available atomic configurations, which can accommodate point defects and compensate for local structural changes induced by radiation. This configurational flexibility enhances the material's ability to self-heal and recover from radiation damage, further contributing to its lower radiation damage radius. This also establishes that HEPy shows a promising characteristic for radiation tolerance. Thus, MD results in this study can be used to optimize the radiation-resistant nature of HEPy by testing other models with orientation and other constituent elements in the composition.



Figure 11. Defect evolution as function time in undoped $Yb_2Ti_2O_7$ and HEPy doped with Y, Gd, and YGdEu at the A sites.

4. Conclusions

Ytterbium titanate pyrochlore oxides with different compositions and high-entropy pyrochlores significantly expand the studied ceramics for the immobilization of Low-Level Radioactive Waste (LRW) ensuring better waste containment and optimizing storage solutions. Studying radiation resistance and the defects formation mechanism is crucial for designing pyrochlore for Radioactive Waste (RW) immobilization materials. Moreover, analyzing the crystal structure of the high-entropy pyrochlores under various conditions helps to understand any changes due to radiation environments. High-entropy pyrochlores contain multiple elements, potentially providing a greater capacity to accommodate and immobilize various radioactive isotopes through diverse interactions.

Molecular dynamics simulations were performed to study the effect of displacement cascades in ytterbium titanate oxide $(Yb_2Ti_2O_7)$ and high-entropy alloys. Calculations were made for equilibrium lattice constant pyrochlore oxides. The displacement cascades in $Yb_2Ti_2O_7$ with Yb, Ti, O of 1 keV, 2 keV, 5 keV, and 10 keV along [100], [110], and [111] were used to determine the threshold energy (E_d) on the radiation damage response of pyrochlore. The effect of displacement cascades on the formation of high-entropy pyrochlore YbYTiZrO₇, YbGdTiZrO₇, Yb_{0.5}Y_{0.5}Eu_{0.5}Gd_{0.5}TiZrO₇, and Yb₂Ti₂O₇ was compared to analyze the radiation stability. The displacement cascades of different incident PKA displayed

that the number of defects is proportional to the incident energy. Higher incident angles have a lower number of defects. The position and inclination angle of the incident angle are important in determining the surviving defects. The defects morphology of HEPy was compared with $Yb_2Ti_2O_7$.

Our study will provide valuable insight and contribute to the advancement of nuclear waste materials. High-entropy pyrochlores offer a broader range of compositions and structures, which could make them more versatile for different nuclear applications. This versatility allows you to fine-tune the material properties based on the application's requirements. High-entropy pyrochlores are still a relatively new area of research and it requires an innovative material design approach. We still believe that more extensive research is required to explore their behavior under radiation and in nuclear environments.

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