

THE MONTE CARLO FLUKA SIMULATION OF GAMMA-RAY AND NEUTRON ATTENUATION CHARACTERISTICS OF REFRACTORY HIGH ENTROPY ALLOYS

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Abstract

In this work, the γ -ray and thermal neutron shielding properties of high entropy alloys in formula $W_x(\text{TaVZr})_{100-x}$, where ($x = 5, 10, 15, 20$ and 25% wt) have been studied. The mass attenuation coefficients (μ_m) for γ -ray of these high entropy alloys have been obtained at energy range 59.6-1332 keV using Phy-X software and FLUKA Monte Carlo code simulation. The obtained results are found to be in good agreement. The W25 for high entropy alloys sample showed the highest μ_m value and the lowest HVL, MFP and transmission factor compared with the other ones in these high entropy alloys samples. As for the case of thermal neutron shielding properties, the FLUKA Monte Carlo code was used for simulated. It was found that W5 high entropy alloy sample shown the highest mass attenuation coefficients (μ_m) value. These results indicated that the high entropy alloys sample, with high W content possesses excellent γ -ray shielding properties, while alloys with low W content possesses superb thermal neutron shielding.

Keywords: FLUKA, High entropy alloys, Gamma-ray, Neutron, Shielding

Introduction

Conflicts over the amount of carbon emissions into the atmosphere and carbon removal that result from rapid economic and industrial expansion are increasingly visible (Pitike *et al.*, 2022; Cheng *et al.*, 2023). Nowadays, fossil fuels remain one of the

most important sources of energy. Yet, it causes serious environmental contamination issues. Thus, it is critical to creating new energy sources, such as geothermal, nuclear, wind, tidal, and solar energy. One of the new energies that are currently employed

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most commonly due to its cheap net cost, great energy density, and lack of pollutants, nuclear energy has some benefits (Natarajan *et al.*, 2020; Zhang *et al.*, 2021). However, the harsh environments in nuclear reactors are not only high temperatures, stress and corrosion but also high levels of ion and neutron radiation for advance nuclear power stations (Ren *et al.*, 2020).

Refractory high entropy alloys (HEAs) were a brand-new high entropy alloy that Senkov *et al.* created and developed in 2011 (Senkov *et al.*, 2011). They are usually composed of five or more metal elements in equal or nearly equal atomic ratios. It has been investigated and proven by numerous researchers that refractory high entropy alloys exhibit a variety of features, which possess qualities superior to those of conventional high entropy alloys, including high strength (Senkov *et al.*, 2011; Han *et al.*, 2017; Li *et al.*, 2022), high plasticity (Senkov *et al.*, 2011; Lee *et al.*, 2018; Zhang *et al.*, 2020), high oxidation resistance, high corrosion resistance (Bachani *et al.*, 2020; Fu *et al.*, 2021), high radiation resistance (Lu *et al.*, 2016; 2019; Sadeghilaridjani *et al.*, 2020), and excellent wear resistance (Chuang *et al.*, 2011; Poletti *et al.*, 2017). Refractory high entropy alloys are employed in nuclear power reactors because of their superior characteristics. The W, Nb, Ta, Ti, V, Cr, Zr, and Hf are the primary refractory elements used in the creation of refractory high entropy alloys.

Research on refractory high entropy alloys based on low-activation elements is now being developed for application in Gen-IV fission and fusion nuclear power reactors (Ayyagari *et al.*, 2018; Kareer *et al.*, 2019; Carruthers *et al.*, 2021; Tan *et al.*, 2022). Yet, high activation elements like Mo and Nb are included in the majority of today's refractory high entropy alloys. Due to their vulnerability to radiation damage, these refractory high entropy alloys cannot be employed as structural materials for nuclear power or in connection with other radioactive applications. Later, in 2022, Ma *et al.* 2022a created and investigated a refractory high entropy alloy with low activation as the primary component (WTaHfTiZr). It has been found that this refractory high entropy alloy exhibits excellent mechanical properties. As a result, it is clearly evident that this refractory high entropy alloy is suitable for nuclear power engineering applications, such as nuclear reactors.

Although a variety of refractory high entropy alloys have had their characteristics examined recently for usage in structural nuclear power applications (Xian *et al.*, 2017; Ayyagari *et al.*, 2018; Yao *et al.*, 2018; Zhang *et al.*, 2018; Kareer *et al.*, 2019; Carruthers *et al.*, 2021; Ma *et al.*,

2022b; Tan *et al.*, 2022). The radiation attenuation characteristics of refractory high entropy alloys are one of the significant aspects that still need to be investigated. Gamma rays and neutrons produced as a result of these nuclear processes are harmful to the environment and those working there (Sriwongsa *et al.*, 2022). It might also have an impact on the service life and cracking of refractory high entropy alloys. The radiation shielding or attenuation properties of refractory high entropy alloys that will be used in nuclear power plants, particularly in nuclear reactors, must be investigated. In this study, the gamma-ray and neutron attenuation properties were examined using FLUKA Monte Carlo simulation. Mass attenuation coefficients, gamma-ray and thermal neutrons transmission factors are the variables to be examined. Based on radiation shielding tests at high-energy particle accelerators, FLUKA was used to study particle interactions and transmission codes (Ferrari *et al.*, 2005; Battistoni *et al.*, 2007). The experimental cross-sectional data (ENDF/B, JEF, JENDL, etc.) are used to guide the performance of various groups of algorithms for the thermal neutron transmission analysis at 0.025 keV energy in this work. The alloys under examination are low-activation alloys made of the refractory elements are W, Ta, V, and Zr (Zhang *et al.*, 2022) that exploited for structural purposes in nuclear fusion power plants. Nuclear fusion power plants are highly anticipated to generate electricity, in other words, the energy of the future. Among these elements, W is the element with the highest metal melting temperature ($T_m = 3695$ K) among them, making it perfect for structural use in nuclear power plants (Hasegawa *et al.*, 2016, El-Atwani *et al.*, 2019, Wu, 2019).

In this context, the $W_x(TaVZr)_{100-x}$ high entropy alloys, where ($x = 5, 10, 15, 20$ and 25 %wt) were simulated for the γ -ray shielding properties using FLUKA Monte Carlo code. The characteristics that needed to be examined were the mass attenuation coefficient (μ_m), half value layer (HVL) and mean free path (MFP). While, ^{241}Am , ^{22}Na , ^{133}Ba , ^{137}Cs , and ^{60}Co are the radiation sources to simulate a radiation transmission event. In addition, thermal neutron shielding properties were also simulated from the FLUKA Monte Carlo code to cover applications in practice.

Materials and Methods

The chemical compositions and density of the high entropy alloys in formula $W_x(TaVZr)_{100-x}$, where ($x = 5, 10, 15, 20$ and 25 %wt) are shown in Table 1 (Zhang *et al.*, 2022).

Table 1. Chemical composition and density of high entropy alloys

Samples	Weight Fraction of Elements (%wt)				Density (g/cm ³)
	W	Ta	V	Zr	
W5	0.050	0.317	0.317	0.317	10.14
W10	0.100	0.300	0.300	0.300	10.56
W15	0.150	0.283	0.283	0.283	10.99
W20	0.200	0.267	0.267	0.267	11.42
W25	0.250	0.250	0.250	0.250	11.85

Gamma-ray interaction

The mass attenuation coefficients (μ_m) express the probability of interaction of γ -ray with the interacting medium. The μ_m of the high entropy alloys were derived from Phy-X software for γ -ray energy range 356–1332 keV using the following equation (Sriwongsa *et al.*, 2022).

$$\mu_m = \sum_i w_i (\mu_m)_i \quad (1)$$

where $(\mu_m)_i$ is the mass attenuation coefficient for the i^{th} element and w_i is the weight fraction of the i^{th} element in the mixture.

Half value layer (HVL) is defined as the thickness of the sample that reduces the γ -ray intensity to half of its initial intensity and can be

calculated from equation the linear attenuation coefficient (μ) by using in equation (Sriwongsa *et al.*, 2022).

$$\text{HVL} = \frac{0.693}{\mu} \quad (2)$$

Mean free path (MFP) is average distance between two successive interactions of γ -ray in medium and simulated from equation (Sriwongsa *et al.*, 2022).

$$\text{MFP} = \frac{1}{\mu} \quad (3)$$

FLUKA Monte Carlo

FLUKA (FLUKtuierende KAskade) is favors used in particle-nuclear sciences. It is mainly in high energy experimental physics and engineering shielding. In this work, the FLUKA Monte Carlo code version 2011.2x-4 which schematic set up for simulate γ -ray and thermal neutron were exhibited in Figure 1 and Figure 2. The simulation for μ_m of material samples can be follows in equation (Issa *et al.*, 2018, Almuqrin *et al.*, 2021).

$$I = I_0 e^{-\mu x} \quad (4)$$

$$\mu_m = \frac{\mu}{\rho} \quad (5)$$

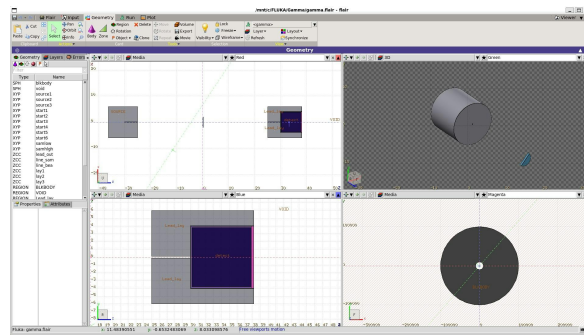


Figure 1. The schematic set up to simulate γ -ray

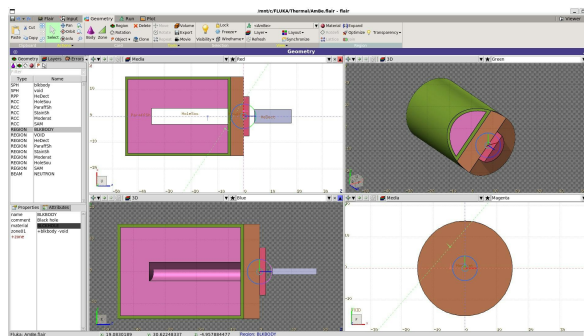


Figure 2. The schematic set up to simulate thermal neutron

where I and I_0 are γ -ray and thermal neutron intensity passed through with and without shielding material, respectively, and x is thickness of sample.

The simulation for thermal neutron shielding has been simulated at the numbers 10^8 of thermal neutrons which is a large enough value for studying trend values (Battistoni *et al.*, 2016).

Results and Discussion

Gamma-ray shielding properties

The mass attenuation coefficient (μ_m) for high entropy alloys samples at thickness 0.2 cm was simulated at γ -ray energy range 59.6–1332 keV. The ^{241}Am (59.6 keV), ^{22}Na (511 and 1275 keV), ^{133}Ba (356 keV), ^{137}Cs (662 keV), and ^{60}Co (1173 and 1332 keV) are the radiation sources to simulate a radiation transmission event as exhibited in Figure 3. It can be seen that the γ -ray at energy range 59.6–356 keV, the value of μ_m increased with increasing W content, but above 356 keV these high entropy alloys properties are not good shielding anymore according to the main of photoelectric effect (PE) process at low energy ranges where the PE probability is excellent. While, the results in Figure 3 shown the value of μ_m at energy range 600–1332 keV have the same tendency of increasing μ_m value with these high entropy alloys. These results according to the density of these high entropy alloys (Sayyed *et al.*, 2018).

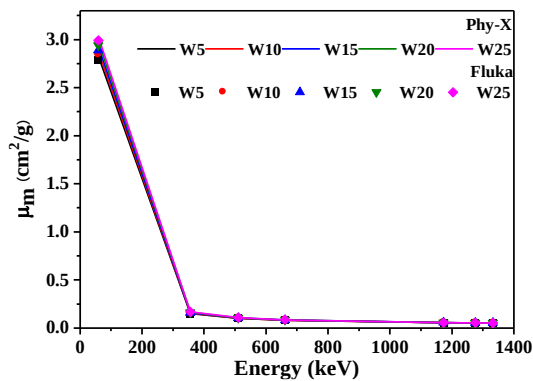


Figure 3. The mass attenuation coefficient of HEA samples

The HVL and MFP values of the high entropy alloys samples is shown in Figure 4 and Figure 5. It was found that both values were low in the PE region and gradually become independent of photon energy in the Compton scattering and pair-

production region. It is to be noted that the W25 alloy sample requires a thinner thickness compared with the other alloy samples in the entire region of interest of the energy. The W25 alloy sample shows a lower HVL and MFP values compared with the other alloy samples. Therefore, it can be concluded that the W25 alloy sample is better at radiation shielding than the other alloy samples. The variation in the HVL and MFP of the alloys is dependent upon the densities which the W25 alloy sample has the largest density. The comparison HVL and MFP values for alloy samples with hematite-serpentine concrete as exhibited in Figure 4. It found that both values for all alloy samples were lower than the hematite-serpentine concrete. It indicated that this alloy series are photon shielding better than the hematite-serpentine concrete (Bashter, 1997; Sriwongsa *et al.*, 2020).

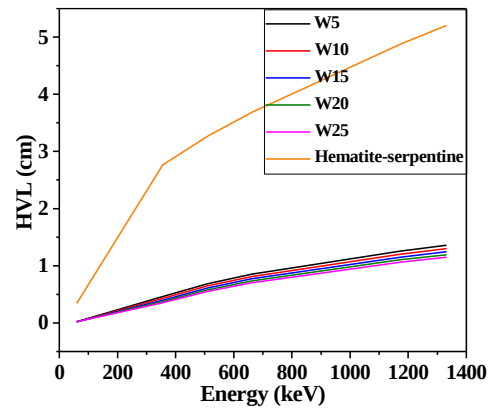


Figure 4. The comparison HVL of HEA samples with hematite serpentine concrete

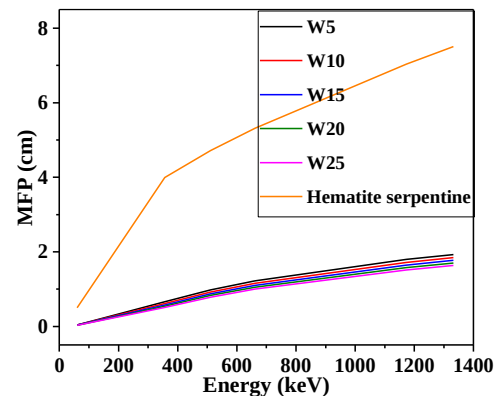


Figure 5. The comparison MFP of HEA samples with hematite serpentine concrete

The transmission factor (TF) is an important factor related to γ -ray penetration. Figure 6 exhibited TF with the energy for the high entropy alloys at a thickness of 0.5 cm. Clearly, the TF values increase, raising the energy between 59.6 to 356 keV. This increase in TF is associated with decrease in the PE interaction and initiation of the Compton scattering (CS) interaction with increasing γ -ray energy. Therefore, the interaction involves a little loss of γ -ray energy, and the γ -ray has enough energy to escape from the thickness of high entropy alloy. In addition, it was found that W25 alloy sample had the lowest TF. It indicated that this alloy sample had excellent γ -ray shielding (Al-Saeedi *et al.*, 2022; Tekin *et al.*, 2022).

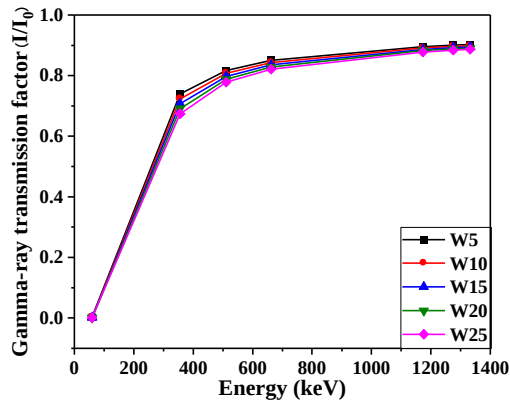


Figure 6. Gamma-ray transmission factor of HEA samples

Thermal neutrons shielding properties

The relationship between the mass attenuation coefficient (μ_m) for thermal neutron and high entropy alloys at a thickness of 2 cm as shown in Figure 7. The trend of μ_m value decreased with increasing W concentration. It means that thermal neutron shielding property decreased with increasing W content (Kaewjaeng *et al.*, 2021).

The effects of the thickness of materials on the thermal neutron shielding properties are shown in Figure 8. The transmission factor values decreased with increasing material thickness for the same W content. Typically, a thicker thermal neutron shield is always more desirable as more collisions can occur between the material and the incoming thermal neutron. This means that more incoming thermal neutrons are absorbed by thicker material due to the higher W atoms per unit area that can interact with incoming thermal neutron in thicker materials. These results in greater absorption of thermal neutron, and improved the thermal neutron shielding abilities of materials (Tiamduangtawan

et al., 2020). Finally, the % statistical error of the simulation at the numbers 10^8 of thermal neutrons which is a large enough value for studying trend values (Battistoni *et al.*, 2016).

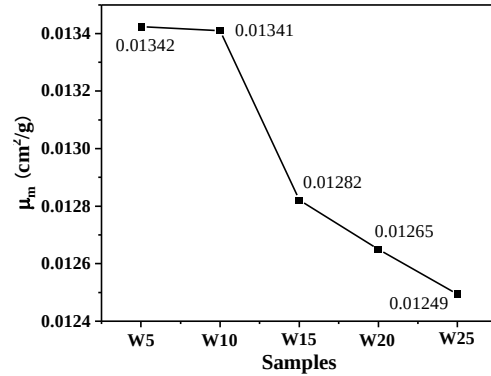


Figure 7. The mass attenuation coefficient for each thermal neutron of HEA samples

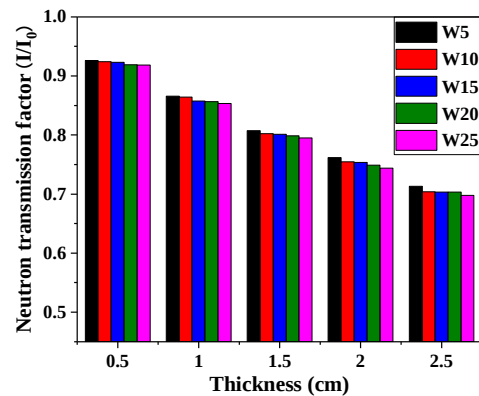


Figure 8. Neutron transmission factor of each HEA samples at thicknesses 0.5-2.5 cm

Conclusions

The available results of the study shielding properties for γ -ray and thermal neutron of the high entropy alloys samples. The results found that the addition of W into high entropy alloys, the μ_m values increased whereas HVL, MFP values and transmission factor decreased. These results indicated that the sample in this work that contains high W content at 25%wt was the excellent shielding γ -ray. For the thermal neutron shielding properties, it can be seen that the sample with low W content at 0.05 wt% showed the highest for thermal neutrons factor at the same thickness and decreased with increasing thickness. These results

indicated that this high entropy alloys which high W content possesses excellent γ -ray whereas low W content possesses superb thermal neutron shielding. Finally, it can be concluded that high entropy alloys are the better choice to traditional lead-based compounds as γ -ray and thermal neutrons shielding materials and hence apply to a range of shielding fields.

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