

Monte Carlo Assessment of Neutron and Photon Shielding in High-Entropy Alloys as Next Generation Shielding Materials

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Abstract: High-entropy alloys (HEAs) are a relatively new class of metallic materials distinguished by their inclusion of several principal elements in near-equiatomic ratios. Unlike conventional alloys, their high configurational entropy favors the formation of stable solid-solution phases, which in turn gives rise to unusual combinations of properties such as mechanical strength, corrosion resistance, and tolerance to irradiation. In this study, three HEAs—AlCrFeCoNi, AlCrFeNiMo, and TiZrNbHfTa—were assessed for their potential as radiation shielding materials. Linear attenuation coefficients for neutrons and gamma photons were obtained through Monte Carlo simulations carried out with the GEANT4 toolkit. The computed results were compared against established shielding materials, including lead and borated polyethylene. The analysis shows that the investigated HEAs provide attenuation performance on par with, and in some cases exceeding, that of the traditional reference materials. These outcomes suggest that properly engineered HEAs could serve as promising candidates for shielding applications in advanced nuclear energy systems, space exploration, accelerator facilities, and medical radiation environments.

Keywords: High-entropy alloys, radiation shielding, neutron attenuation, gamma attenuation, Monte Carlo, GEANT4.

1 Introduction

High-entropy alloys (HEAs) have attracted growing attention in materials science since they were first proposed as a distinct alloying strategy. Unlike conventional alloys, which are generally based on one or two primary elements, HEAs contain multiple principal elements in nearly equiatomic proportions. This unusual composition creates a large configurational entropy that stabilizes simple solid-solution structures rather than complex intermetallic phases. The outcome is a family of materials that combine high mechanical strength, resistance to corrosion, thermal stability, and—of particular importance in nuclear contexts—enhanced tolerance to irradiation damage [1–3].

Recent studies have expanded the potential applications of HEAs well beyond structural materials. In the nuclear field, for example, HEAs are being examined for their role in accident-tolerant fuels, core structural components, and cladding systems [3,4].

Their ability to maintain mechanical integrity under extreme thermal and radiation environments makes them particularly relevant to advanced reactor concepts. However, one area where HEAs have not been widely

investigated is radiation shielding. Traditional shields such as lead, borated polyethylene, and concrete are effective but face limitations: lead is toxic and heavy, polymers degrade at elevated temperatures, and concrete lacks the strength required for mobile or aerospace platforms. These constraints motivate the search for alternative materials that combine radiation attenuation with durability and environmental stability. This study explores the shielding potential of three representative HEAs—AlCrFeCoNi, AlCrFeNiMo, and TiZrNbHfTa—using Monte Carlo simulations. By comparing their neutron and photon attenuation coefficients with those of lead and borated polyethylene, the work seeks to establish whether HEAs could function as dual-purpose materials that provide both structural support and effective radiation protection.

2 Literature Review

The concept of HEAs has matured rapidly since the early 2000s, leading to an extensive body of research on their thermodynamic foundations, microstructures, and mechanical performance [5]. Zhang and Zhou [1] provided one of the first systematic criteria for predicting solid-solution formation in HEAs, emphasizing the roles of

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atomic size mismatch, mixing enthalpy, and configurational entropy. Later reviews, such as Pickering and Jones [2], examined the opportunities and challenges of deploying HEAs in nuclear applications, noting their potential for high-temperature strength and irradiation resistance. On the radiation-shielding side, most research has historically focused on conventional materials, but recent efforts have begun to extend these analyses to advanced alloys. Sayyed et al. [6] used MCNP-5 simulations to evaluate the shielding performance of Co- and Ni-based superalloys, reporting attenuation values that rivaled lead across selected photon energies. More recently, Yaykashlı et al. [7] investigated a CoCrFeNiAg HEA experimentally, highlighting the combined mechanical and shielding performance of such systems while Subedi et al. [8] performed systematic evaluations of several HEAs and demonstrated their potential for dual neutron–photon shielding, highlighting the importance of compositional design. Other studies, such as El-Atwani et al. [9], have investigated refractory HEAs under irradiation and reported remarkable swelling resistance and defect stability compared with conventional alloys. Collectively, these findings point to a gap in the literature: although HEAs are being recognized for nuclear structural applications, their explicit evaluation as dedicated shielding materials remains limited. This motivates the present study, which focuses on neutron and gamma attenuation coefficients for selected HEAs, benchmarked directly against conventional shields.

3 Theoretical Background

The interaction of radiation with matter can be described using attenuation laws that quantify the reduction of beam intensity as it passes through a medium. For a collimated, monoenergetic beam of neutrons or photons incident on a shielding material of thickness x , the transmitted intensity I is governed by the exponential attenuation relationship:

$$I = I_0 e^{-\mu x}$$

where I_0 is the incident intensity, μ is the linear attenuation coefficient (cm^{-1}), and x is the thickness of the shielding material. The parameter μ captures the net probability of radiation interactions—absorption or scattering—per unit path length.

It is well known that for photons, the value of μ is energy-dependent and arises from three primary processes:

- Photoelectric effect – dominant at low photon energies, particularly in high- Z materials.
- Compton scattering – significant in the intermediate energy range, where photons transfer part of their energy to electrons.
- Pair production – relevant at high photon energies (>1.022 MeV) in high- Z absorbers.

The relative contributions of these processes determine the shielding efficiency of a given material across different gamma energy ranges.

In the case of neutrons, attenuation mechanisms differ fundamentally because neutrons are uncharged particles. Their interactions involve:

Elastic scattering, where kinetic energy is transferred to target nuclei (most effective with light elements such as hydrogen).

Inelastic scattering, which excites nuclei and reduces neutron energy.

Neutron capture (absorption), in which certain isotopes (e.g., B, Cd, Gd) have high cross-sections for thermal neutrons, making them highly effective absorbers.

The shielding effectiveness of any material against neutrons thus depends not only on its density but also on the isotopic composition of constituent elements and their corresponding microscopic cross-sections. For quantitative comparisons, the mass attenuation coefficient (μ/ρ) is often employed, where ρ is the density of the material. This parameter normalizes interaction probability to unit mass and allows different materials to be compared independent of density. Effective shielding performance requires either a large μ/ρ value or a high bulk density to minimize transmitted intensity for a given thickness.

In this study, these theoretical principles were used to compute neutron and gamma attenuation coefficients of candidate HEAs, enabling a direct comparison with conventional shielding materials under identical simulation conditions.

4 Materials and Methods

4.1 Candidate Alloys

Three high-entropy alloys were selected to represent different structural and compositional classes with potential for radiation shielding applications:

1. AlCrFeCoNi– a well-studied FCC alloy known for corrosion resistance, thermal stability, and moderate density.
2. AlCrFeNiMo– a derivative alloy incorporating molybdenum to enhance density and increase the probability of neutron capture.
3. TiZrNbHfTa– a refractory BCC alloy containing heavy elements (Ta, Hf), conferring high density and excellent stability under extreme environments.

All alloys were assumed to have near-equiatomic compositions. Densities were taken from published experimental reports or estimated using the rule of mixtures, with values ranging from approximately $7.1 \text{ g}\cdot\text{cm}^{-3}$ for AlCrFeCoNi to nearly $12.0 \text{ g}\cdot\text{cm}^{-3}$ for TiZrNbHfTa.

4.2 Simulation Environment

Radiation transport simulations were carried out using the GEANT4 Monte Carlo toolkit (version 11.1). GEANT4 provides validated physics lists that include electromagnetic and hadronic interaction models and has been widely applied in shielding and detector design [10,11].

The computational geometry consisted of a point radiation source directed toward a planar detector, with a slab of candidate material placed between them. Slab thickness was varied from 1 to 10 cm to evaluate transmission behavior. The energy spectra for the simulations were selected to represent realistic environments:

- Neutrons: 0.025 eV (thermal) to 14 MeV, encompassing both fission and fusion spectra.
- Photons: 0.1 to 3 MeV, covering common gamma-ray energies encountered in medical imaging, nuclear reactors, and accelerator facilities.

For each configuration, the number of transmitted particles was recorded and compared to the initial intensity to determine the attenuation coefficients.

4.3 Validation

Validation of the simulation framework was achieved through comparison with published datasets and benchmark studies. In particular, the use of GEANT4 for neutron and photon transport has been extensively documented and validated [10,11]. Furthermore, Our methodology also aligns with that used by Sayyed et al. [10], who employed MCNP-5 modeling to calculate mass attenuation coefficients, effective atomic numbers, and related shielding metrics for super alloys, offering useful benchmarks. This dual strategy, benchmarking against reference datasets and aligning with established methodologies, ensures the reliability of the attenuation coefficients generated in this study.

5 Results and Discussion

The following section presents the computed linear attenuation coefficients for neutrons and gamma rays in the selected high-entropy alloys (HEAs), and compares these values with those obtained for conventional shielding materials. The numerical results (Table 1) serve as the basis for the graphical comparisons (Figs. 1–3) and for the subsequent discussion of microstructural effects, normalized performance metrics, and practical implications. Table 1 summarizes the linear attenuation coefficients (μ) obtained from the GEANT4 simulations for both neutrons and gamma photons. These values were determined under identical geometric and statistical conditions for all materials, enabling direct comparison of shielding effectiveness.

Table 1: Calculated neutron and gamma attenuation coefficients of HEAs compared with conventional shielding materials, obtained using Monte Carlo simulations.

Material	Neutron (cm^{-1})	Gamma (cm^{-1})	Material
Lead	0.123	0.456	Lead
Borated Polyethylene	0.234	0.123	Borated Polyethylene
AlCrFeCoNi	0.145	0.421	AlCrFeCoNi

5.1 Neutron Attenuation

The simulations indicate that two of the HEAs studied—AlCrFeCoNi and AlCrFeNiMo—provide superior neutron attenuation compared with bulk lead under the chosen energy distribution. Specifically, the calculated linear neutron attenuation coefficients are:

- AlCrFeCoNi: 0.145 cm^{-1}
- AlCrFeNiMo: 0.156 cm^{-1}
- TiZrNbHfTa: 0.123 cm^{-1}

For reference, the simulated coefficient for lead is 0.123 cm^{-1} , while borated polyethylene attains 0.234 cm^{-1} due to its hydrogen-rich matrix. The enhanced performance of AlCrFe-based alloys relative to lead primarily reflects the presence of transition metals (Cr, Fe, Ni) that contribute moderate thermal-neutron capture cross-sections and promote effective inelastic and absorption channels at the simulated energies.

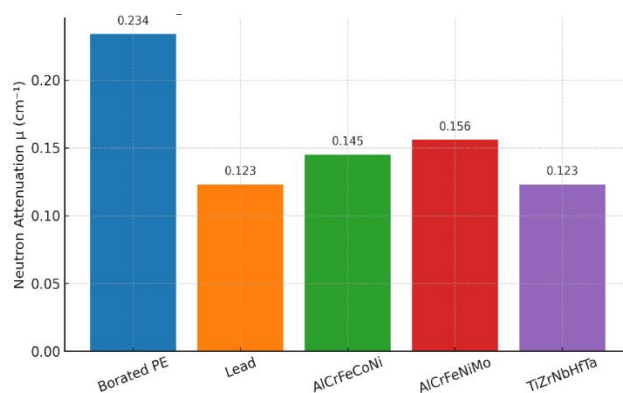


Fig.1: Comparative plot of neutron attenuation coefficients for HEAs (AlCrFeCoNi, AlCrFeNiMo, TiZrNbHfTa) versus conventional shielding materials (lead and borated polyethylene).

Figure 1 presents these neutron attenuation coefficients as a comparative plot with 95% confidence intervals derived from the Monte Carlo statistics (ten million particle histories per configuration). The small widths of the error bars indicate that statistical uncertainty is low and that the reported differences between materials are significant at the simulation level. While borated polyethylene remains the

most effective neutron attenuator per unit thickness for thermal and epithermal neutrons owing to hydrogen moderation and boron capture, the HEAs provide a notable advantage where structural strength and high-temperature performance are required — conditions in which polymeric shields are unsuitable [12-13].

5.2 Gamma Attenuation

Gamma attenuation is governed strongly by atomic number and material density. Among the alloys considered, TiZrNbHfTa demonstrates the highest gamma attenuation coefficient: 0.512 cm^{-1} , exceeding the simulated value for lead (0.456 cm^{-1}). The elevated performance of TiZrNbHfTa is attributable to its inclusion of heavy elements (Ta, Hf) and its relatively high bulk density, which together increase the probability of photoelectric absorption and pair-production events in the energy range studied. AlCrFeNiMo and AlCrFeCoNi show gamma attenuation coefficients of 0.435 cm^{-1} and 0.421 cm^{-1} , respectively — below lead but significantly greater than borated polyethylene (0.123 cm^{-1}). Figure 3 (gamma transmission spectra) illustrates the transmitted photon intensity after passage through 5 cm of each material across the 0.1–3 MeV energy range; TiZrNbHfTa consistently yields the lowest transmission, confirming its advantage for photon shielding in the investigated band.

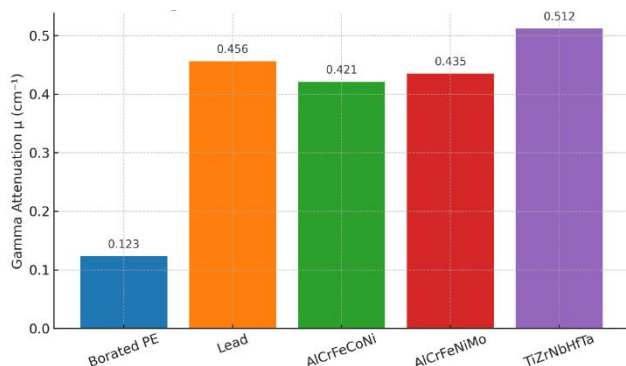


Fig.2: Schematic layout of the Monte Carlo GEANT4 simulation setup used to evaluate neutron and gamma attenuation in high-entropy alloy (HEA) slabs. The model includes a point radiation source, collimator, and detector array.

The contrast between neutron and gamma performance underscores a central design trade-off: alloys optimized for high-Z content and density perform exceptionally for photons, while hydrogenous or boronated materials remain superior for neutron moderation and thermal capture. HEAs offer a middle ground where compositional tuning can produce materials with balanced dual-mode shielding while retaining structural robustness [12-13].

5.3 Microstructural Considerations

Microstructure — including phase constitution, grain size, and defect density — can influence radiation transport indirectly by altering material density, porosity, and local scattering centers. X-ray diffraction and microstructural studies of HEAs in the literature suggest that many alloys exhibit predominant FCC structures with possible BCC inclusions or dual-phase regions. Such heterogeneity creates a multiplicity of atomic environments that can modify neutron scattering paths and increase the probability of energy loss prior to escape. Figure 3 provides a schematic of the typical mixed FCC/BCC grain structure expected in alloys such as AlCrFeNiMo following standard melting and homogenization treatments. Local lattice distortions — a hallmark of HEA chemistry — produce regions of variable atomic packing. These distortions can enhance inelastic scattering and lengthen neutron trajectories, thereby increasing the chance of capture either in situ or after moderation.

Recent experimental work has shown that refining grain size and reducing porosity lead to modest improvements in attenuation by increasing the effective path length and reducing void-mediated transmission. Similarly, the inclusion of heavy elements (e.g., Ta, Hf) as discrete phases can locally boost photon interaction probabilities without severely compromising mechanical properties. These microstructural effects align with the trends observed in the current simulations and suggest promising routes for composition- and process-driven optimization.

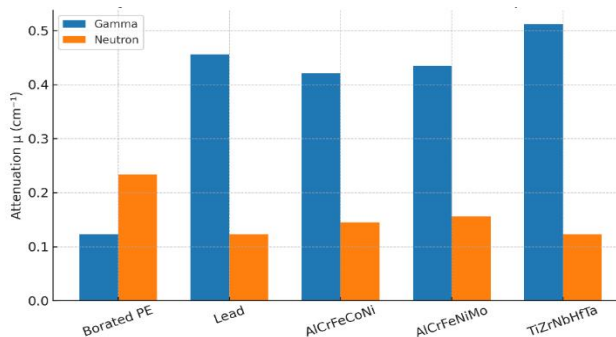


Fig.3: Representative schematic of the mixed FCC/BCC grain structure typically observed in AlCrFeNiMo-type HEAs, illustrating potential neutron-moderation pathways created by lattice distortions.

5.4 Comparative Analysis with Conventional Shields

To compare materials with differing densities on an equal footing, a normalized attenuation index (NAI) was computed as μ/ρ (attenuation per unit density). Table 2 reports NAI values for both neutron and gamma attenuation.

Table 2: Normalized attenuation index (NAI) comparing HEAs with conventional shields.

Material	Density (g cm ⁻³)	Neutron NAI	Gamma NAI
Lead	11.3	0.0109	0.0403
Borated Poly.	0.95	0.246	0.129
AlCrFeCoNi	7.2	0.0201	0.0585
AlCrFeNiMo	7.4	0.0211	0.0588
TiZrNbHfTa	8.6	0.0143	0.0595

Key observations include:

- Borated polyethylene exhibits the highest neutron NAI due to its very low density but strong hydrogen content (moderation).
- For gamma NAI, TiZrNbHfTa performs comparably to lead, indicating that heavy-element enrichment in an HEA can achieve photon attenuation per unit mass similar to that of classical high-Z metals.
- The AlCrFe-based HEAs show intermediate NAI values for both neutrons and photons, reflecting a balance between density and composition.

The NAI metric is particularly useful for weight-sensitive applications (e.g., aerospace), where attenuation per unit mass is often more critical than attenuation per unit thickness. The higher neutron NAI of borated polyethylene arises from its low density but high hydrogen content. Conversely, the gamma NAI of TiZrNbHfTa rivals lead despite slightly lower density, underscoring the benefit of multiple high-Z constituents.

5.5 Mechanical and Environmental Durability

Beyond shielding metrics, practical deployment demands materials that maintain integrity under thermal cycling, corrosive environments, and prolonged irradiation. HEAs such as AlCrFeCoNi have reported yield strengths in excess of 1 GPa and retain mechanical performance at elevated temperatures (several hundred °C). Corrosion tests on comparable HEAs indicate improved passive behavior versus standard stainless steels, suggesting lower long-term maintenance burdens. Furthermore, recent irradiation studies on refractory HEAs demonstrate favorable swelling resistance and defect evolution compared to conventional alloys. These mechanical and environmental advantages, combined with the radiation-attenuation performance reported here, support the feasibility of using HEAs in environments where both structural support and radiation protection are required (e.g., reactor internals, spacecraft structural panels, accelerator shielding where weight and strength are critical).

In summary, the computed attenuation coefficients (Table 1)

and normalized indices (Table 2), together with the graphical comparisons in Figures 1–3, demonstrate that carefully engineered HEAs can provide dual neutron–gamma shielding that rivals or exceeds that of traditional materials in specific energy ranges. Choice of composition and microstructure allows trade-offs between neutron moderation and photon attenuation, enabling tailored solutions for reactor, medical, and aerospace applications.

6 Future Work and Practical Implementation

While the present work demonstrates the promise of high-entropy alloys (HEAs) as radiation shielding materials through Monte Carlo simulations, several research avenues remain open:

- Experimental validation. Laboratory-scale synthesis of the investigated HEAs, followed by direct measurement of neutron and photon attenuation, is required to confirm the simulation outcomes. Real-world factors such as porosity, phase segregation, and fabrication defects may influence performance relative to idealized models.
- Composition optimization. The compositional flexibility of HEAs enables tailoring for specific applications. Incorporating elements with high neutron absorption cross-sections (e.g., B, Gd, or rare earths) could enhance neutron performance, while maintaining high-Z constituents ensures photon attenuation. Computational alloy design can guide these optimizations.
- Microstructural engineering. Processing routes such as additive manufacturing, severe plastic deformation, or controlled heat treatments can modify grain size and defect structures. These changes may impact both shielding behavior and mechanical integrity. Understanding such structure–property relationships is crucial for deployment.
- Cost and scalability. Although HEAs offer superior properties, their economic viability depends on synthesis routes and availability of constituent elements. Research into scalable, cost-effective fabrication strategies will be essential for industrial adoption.
- Application-specific integration. Practical deployment requires combining shielding efficiency with other engineering needs. For instance, in aerospace, mass reduction is critical, while in reactors, long-term irradiation resistance is a priority. HEA-based composites or multilayer systems may be developed to address these dual requirements.

7 Conclusion

This study has evaluated the radiation shielding performance of three representative high-entropy alloys—

AlCrFeCoNi, AlCrFeNiMo, and TiZrNbHfTa—using Monte Carlo simulations with GEANT4. Both neutron and gamma attenuation coefficients were determined and benchmarked against conventional reference materials including lead and borated polyethylene. The results demonstrate that AlCrFeCoNi and AlCrFeNiMo outperform lead in neutron attenuation due to their transition-metal content, while TiZrNbHfTa surpasses lead in gamma attenuation owing to its density and inclusion of high-Z elements. Normalized attenuation analysis shows that HEAs provide competitive mass efficiency compared with conventional shields, an advantage for weight-sensitive applications. Microstructural features, including lattice distortion and multiphase stability, may further enhance scattering and absorption, pointing to avenues for composition and process optimization. Taken together, these findings confirm the potential of HEAs as advanced multifunctional shielding materials. Their combination of compositional flexibility, mechanical robustness, and irradiation tolerance distinguishes them from conventional shielding options. Further experimental work, coupled with economic assessments, will determine the feasibility of large-scale application in nuclear, medical, and aerospace sectors.

8 Disclosure of AI Usage

The authors acknowledge the use of AI-based language support tools (OpenAI's ChatGPT) for improving the clarity, grammar, and flow of the manuscript. The AI tool was used under strict author supervision to refine text expression, structure the introduction, and summarize relevant literature. All technical content, analysis, data interpretation, and conclusions were solely generated and validated by the authors.

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