Multilayer Sensitivity Analysis for new metal hydride Shielding Material

Boravy Muth* and Chang Je Park

Sejong University, 209 Neungdong-ro, Gwangjin-gu, Seoul 143-747, Republic of Korea *Corresponding author: ravy1991@sju.ac.kr

1. Introduction

Determination of radiation shielding material is an important part for the nuclear reactor, a particle detector, spacecraft, other parts of nuclear facilities, and these fields also are related to radiation shielding for radiological material [1]. General shielding materials have effective shielding properties for challenging at high temperature, corrosion in the inclement environment, good radiation effect, as well as the cost of material that need to be carefully selected to provide a long period for their servicing in nuclear facilities [2]. The most advanced and advantageous of neutron shielding for nuclear facilities (nuclear reactor) is the combination of hydrogen-rich materials, heavy metal elements, and some other neutron absorber materials because of the characteristics to slow down the process of inelastic scattering by heavy elements and elastic scattering by hydrogen elements [1] [2]. However, a good candidate shielding material for the gamma radiation should have a high Z element number which gives high photo-electric effect, Compton scattering and pair production. Thus, lead, iron, tungsten, and depleted uranium are widely used as shielding medium for the high radiative gamma radiation source. These days various new and challenging materials are proposed for shielding both neutron and gamma simultaneously. Among them, metal hydrides are good candidates.

In this study, metal hydrides such as Magnesium hydride (MgH₂), Titanium hydride (TiH₂), Zirconium hydride (ZrH₂), and Magnesium iron hexahydride (Mg₂FeH₆) are chosen for evaluation as the neutron and gamma shielding material. These materials contain the hydrogen nuclei performing as an active moderator to slow down the fast neutron and gamma flux [4]. The intensive study of these materials can be found in various useful references for individual materials such as MgH₂ [5], Mg₂FeH₆ [6], TiH₂ and ZrH₂ [3].

In this paper, the exploration of the combination of materials is conducted to find the potential shielding materials suitable for both neutron and gamma radiation. In this case, metal hydride combines with a single element of metal with the high-Z number, and carbide compound elements will be investigated and analyzed their shielding property. All shielding simulation analysis are carried out based on the Monte Carlo code with as simplified model.

2. Code Description

Among various shielding analysis code, the MCNP6 (Monte Carlo N-Particles) is employed for full 3D modeling and calculation that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. In the case of neutron calculation, ENDF/B-VII.1 cross section library is used and for gamma transport analysis, Mcplib84 is used. The MCNP code applies for various applications including radiation protection and dosimetry, radiation shielding, nuclear criticality analysis [7]. In the radiation shielding problem, the general source definition SDEF card in MCNP is implied with F4 card to obtain the surface fluxes at detector region. The simulation conditions are included of 10 MeV of particle energy with 10,000,000 number of particles to obtain the low relative error.

3. Analysis procedures and simulation parameters

3.1. Simulation Condition and Modeling

Fig 1 shows the model of single-layer material and Fig 2 shows the model of multilayer materials. The model is divided into three parts. The first part of the geometry is between -12 cm to 0 cm, the particle is considered to travel in the straight line in x-axis direction at -10 cm before hitting the target materials. The first region contains only air. The second part is the material region for evaluation. The thickness of the material is one of the key parameters. The small box of the third part represents the detector (artificially which contains only air) to detect the amount to particle flux produced after passing through the material region.



Fig 2. Model of multilayers shielding problem

3.2. Analysis procedures3.2.1. Single Layer Analysis

The simulation of single-layer materials is critical to classify the effectiveness of each material for radiation shielding problems. Fig 3 and Fig 4 shows the neutron and gamma flux compared to the energy of particles which are ranged 1 to 10 MeV with 20 cm of target thickness, respectively. Ta and W show very excellent behavior to shield gamma particle completely but did not show the same for neutron case. However, Ta and W are still very effective to shield neutron flux at very high energy compared to other materials.



Fig 5. Neutron flux vs. the target thickness

Fig 5 and Fig 6 display the neutron and gamma flux compared to the target thickness, respectively. As can be seen, the neutron flux shows a very similar trend

among each other. All materials produce the amount of flux around 1E-05 magnitude. In case of gamma irradiation, it shows completely different to neutron irradiation. Noticeable on material such as Ta, W, and Bi show similar behavior to each other but different from the rest, with noticeable of shielding gamma flux completely around 14 cm. This behavior shows completely different from neutron flux.



Fig 6. Gamma flux vs. the target thickness Table 1. Neutron and Gamma flux of single layer material (20 cm thickness, 10 MeV)

Material	Neutron Flux (#/cm ² .s)	Gamma Flux (#/cm ² .s)				
MgH2	2.11E-05	6.63E-05				
TiH2	1.02E-05	3.31E-05				
ZrH2	1.24E-05	1.10E-05				
Mg2FeH6	1.23E-05	4.41E-05				
B4C	1.09E-05	5.64E-05				
SiC	1.60E-05	4.49E-05				
Та	9.12E-06	0.00E+00				
Bi	2.21E-05	2.07E-07				
W	6.80E-06	0.00E+00				

Relative Error = 0.01 to 0.30

3.2.2. Multilayer Analysis

Reference [2] stated that the advanced material for shielding is the combination of hydrogen-rich materials, heavy metal elements, and some other neutron absorber materials. Then, multilayer sensitivity will investigate and carry out the above concept as follows:

• 2 layers of material: 10 cm each, the first layer is Hydride and 2nd layer is Metal or Carbide.

• 4 layers of material: 5 cm each where 1st and 3rd are Hydride, 2nd and 4th are metal or carbide.

 $\bullet~5$ layers of material: 4 cm each where $1^{st},~3^{rd},~5^{th}$ are a hydride, and $2^{nd},~4^{th}$ are metal or carbide.

The energy of this cases will start at 10 MeV. The position of the material can be reversed; however, in this paper, only three cases of multilayer later as mention above will be introduced.

Table 2. Neutron Flux of Multilayer (neutron/cm².s)

MATERIAL	2 LAYERS	4 LAYERS	5 LAYERS
MgH ₂ +B ₄ C	1.50E-05	1.46E-05	1.67E-05
MgH2+SiC	1.75E-05	1.87E-05	2.07E-05
MgH2+Bi	2.15E-05	2.14E-05	2.27E-05
MgH2+Ta	1.61E-05	1.35E-05	1.43E-05
MgH2+W	1.48E-05	1.10E-05	1.26E-05
TiH ₂ +B ₄ C	8.52E-06	1.06E-05	1.09E-05
TiH ₂ +SiC	1.09E-05	1.31E-05	1.33E-05
TiH ₂ +Bi	1.32E-05	1.42E-05	1.42E-05
TiH ₂ +Ta	1.01E-05	9.73E-06	8.62E-06
TiH ₂ +W	9.41E-06	7.78E-06	8.62E-06
ZrH ₂ +B ₄ C	8.93E-06	1.05E-05	1.21E-05
ZrH ₂ +SiC	1.14E-05	1.41E-05	1.47E-05
ZrH ₂ +Bi	1.48E-05	1.60E-05	1.64E-05
ZrH ₂ +Ta	1.11E-05	1.03E-05	1.04E-05
ZrH_2+W	1.12E-05	8.70E-06	9.99E-06
Mg ₂ FeH ₆ +B ₄ C	9.56E-06	1.07E-05	1.20E-05
Mg ₂ FeH ₆ +SiC	1.18E-05	1.40E-05	1.47E-05
Mg ₂ FeH ₆ +Bi	1.49E-05	1.63E-05	1.57E-05
Mg ₂ FeH ₆ +Ta	1.14E-05	1.00E-05	9.79E-06
Mg ₂ FeH ₆ +W	9.84E-06	8.33E-06	8.51E-06

Relative error between = 0.01 to 0.30

Table 3. Gamma Flux of Multilayer (photon/cm².s)

MATERIAL	2 LAYERS	4 LAYERS	5 LAYERS
MgH ₂ +B ₄ C	6.13E-05	6.08E-05	5.98E-05
MgH2+SiC	5.85E-05	5.85E-05	5.54E-05
MgH2+Bi	4.81E-06	5.19E-06	7.90E-06
MgH2+Ta	5.77E-07	7.12E-07	1.80E-06
MgH2+W	2.27E-07	3.83E-07	6.85E-07
TiH ₂ +B ₄ C	4.09E-05	4.33E-05	4.44E-05
TiH ₂ +SiC	3.77E-05	3.91E-05	3.85E-05
TiH ₂ +Bi	2.79E-06	2.70E-06	4.83E-06
TiH ₂ +Ta	3.31E-07	3.62E-07	9.32E-07
TiH_2+W	1.29E-07	3.29E-07	3.31E-07
ZrH ₂ +B ₄ C	2.49E-05	2.55E-05	2.31E-05
ZrH ₂ +SiC	2.02E-05	2.21E-05	1.94E-05
ZrH ₂ +Bi	1.19E-06	1.12E-06	2.07E-06
ZrH ₂ +Ta	1.38E-07	2.24E-07	4.49E-07
ZrH ₂ +W	9.04E-08	6.30E-08	1.98E-07
Mg ₂ FeH ₆ +B ₄ C	4.80E-05	5.04E-05	5.00E-05
Mg ₂ FeH ₆ +SiC	4.60E-05	4.70E-05	4.42E-05
Mg ₂ FeH ₆ +Bi	3.53E-06	3.44E-06	5.49E-06
Mg ₂ FeH ₆ +Ta	4.65E-07	4.75E-07	1.21E-06
Mg ₂ FeH ₆ +W	1.28E-07	3.04E-07	4.27E-07

Relative error between = 0.01 to 0.30

Table 2 and Table 3 depict both neutron and gamma flux at 10 MeV with a target thickness of 20 cm of the multilayer material, respectively. As mention above, 2, 4 and five layers are the candidate for our investigation to find out the effect of madeira shielding capability. The result shows the significant impact on the gamma simulation rather than neutron. ZrH₂ combines with W for different multilayer cases show the huge effect on gamma flux following by ZrH₂ combined with Ta (It doesn't mean ZrH₂, and W or T are mixed singular material, every material in multilayer sensitivity analysis are standalone material in one layer as mention in section 3.2.2). Though, neutron flux of multilayer calculation shows very high flux compared to the gamma with the order approximately of 7E-06 magnitudes. This result can be extended to investigate ten layers of material which consist of hydride, high-Z number metal, and carbide compound, or the combination of a single layer with three different materials as described above.

4. Conclusion

In this paper, the exploration of challenging material to shield neutron and gamma radiation is conducted and investigated based on combining hydride compound with high-Z number metal and carbide material. And the multilayer concept is introduced by placing individual material to the designated location and various possible cases are analyzed based on the simplified MCNP model. The result obtains from the single layer/multilayer material simulation are compared based on the surface flux (n/cm²s). Form the simulation results, it is found that the single layer material shows a significant enhancement for gamma shielding for Ta and W material. However, for neutron shielding, most materials exhibit similar trends without any noticeable effect due to neutron characteristics of materials. Therefore, multilayer with combination of ZrH₂ and W could provide a better shielding performance and it is expected to be applicable various areas for neutron and gamma radiation shielding requirements.

REFERENCES

- J.G. Fantidis, The comparison between simple and advanced shielding materials for the shield of portable neutron sources. Int. J. Radiat. Res., Vol 13, No 4, 2015.
- [2] Huasi Hu, et al., Study on composite material for shielding mixed neutron and gamma-rays, IEEE Transaction on Nuclear Science, Vol. 55, No. 4, 2008.
- [3] M. Hiroaki, et al., Properties of Cold-Pressed Metal Hydride Materials for Neutron Shielding in a D–T Fusion Reactor. Plasma and Fusion research, Vol 10, 2015.
- [4] T. Hayashi, et al., Advanced neutron shielding material using zirconium borohydride and zirconium hydride. Journal of Nuclear Materials Vol. 386-388, Page 119-121, 2009.
- [5] Qian Yu, et al., Size-dependent mechanical properties of Mg nanoparticles used hydrogen storage, 2015. Applied Physics Letters 106, 2015.
- [6] N.A. Niaz, et al., Preparation of Mg₂FeH₆ Nanoparticles for Hydrogen storage properties. Journal of Nanomaterials, Vol 2013, 2013.
- [7] Pelowitz, Denise B. "MCNP6 user's manual version 1.0.", LA-CP-13-00634, Rev. 0, (2013).