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The Properties of Ternary Alloys Protectors Pb-Cu-Te for a Neutral Low Ionization Radiation

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Abstract: The purpose of present research work is evaluation the gamma-ray interactions with five lead-based alloys. The samples were defined with high lead (Pb) content (>99.8%) and doped with trace amounts of copper (Cu) and tellurium (Te). The key shielding parameters were calculated through gamma photon energy ranged (0.05953–1.332)MeV using three computational tools: XCOM, NGCal, and Py-MILBUF. The programs showed excellent agreement, confirming the reliability of the data, with a slight discrepancy in Py-MILBUF at 0.08099 MeV near the K-edge of lead. All parameters, including mass attenuation coefficient (MAC), molecular cross-section (σ_{tm}), and electronic cross-section (σ_{ele}), strongly depended on photon energy, decreasing sharply as energy increased—reflecting a shift from the Photoelectric Effect to Compton Scattering. Sample S3, with the highest lead content (99.93%), exhibited superior shielding, recording the highest MAC, an effective atomic number ($Z_{eff} = 81.974$), and the shortest mean free path (MFP), making it the most efficient shield. Conversely, sample S4, with the lowest lead and highest copper content, showed the weakest shielding. The findings confirm that small compositional changes in lead-based alloys significantly affect shielding performance, with higher lead fractions being critical. These results provide a strong basis for developing advanced shielding materials for nuclear and medical applications.

Keywords: Gamma-ray, Lead Alloys, Mass Attenuation Coefficient, Effective Atomic Number, Mean Free Path, XCOM, NGCal, SAZ Code

1. Introduction

Electrons and neutral particles (like photons) interact with the target substance in ways that overlap. The release of electrons and a collection of electron-positron pairs coincides with the interaction of photons with any object. There are two types of interactions between electrons and materials. They are experiencing Continuous Slowing Down (CSD) as a result of many collisions with the target's atomic electrons. Additionally, they release radiation that diffuses in various ways, which causes them to lose their kinetic energy. Photon-medium interactions are seen as statistical processes. Quantum mechanical statistical phenomena regulate all experimental functions, which may be seen as continuous deterministic operations at the minuscule level. Without any interaction, a photon may go an infinite distance. The photon disappears from the incident beam as it interacts, causing the beam's intensity to decrease. the sign that a photon's intensity is being absorbed by interactions inside a material instead of kinetic energy loss. The distance a photon traveled before arriving at the research region has no bearing on the

likelihood that it would interact inside a medium dx . This feature suggests that the intensity of the incoming photon beam will drop exponentially [1-4].

Many researchers are drawn to the subject of neutron protection, particularly when they are interested in themes related to radiation damage and risks or when they are searching for applications in science and technology. While charged particles and photons share many characteristics, neutrons have particular characteristics that are exclusive to their interactions with any target substance. Neutron slowing down is the process by which neutrons lose energy through many elastic collisions as they go through the material, just like charged particles do. Since the neutron is diffracted off its original course and has a lower kinetic energy after scattering, their interactions with matter are comparable to those of charged particles. Neutrons don't leave any ionization trails behind them, in contrast to charged particles. They may also travel great distances without interacting and be absorbed in a single encounter, which is comparable to photon propagation. Over a broad range of energies, confined neutrons interact with atomic nuclei. This approach differs from interactions between charged particles and photons, where interactions with atomic electrons are the primary source of energy loss or absorption. Since neutrons are tiny, heavy, and electrically neutral, they may enter atoms' deep cores even with modest kinetic energy. They also approach the nucleus and are easily absorbed by it. The process of absorption called exoergic. It followed by the emission of neutral radiation, often charged particle [5].

Historically, materials like concrete, water, and glass have been used for shielding, but high-density and high-atomic-number materials such as lead (Pb) ($Z = 82$, density $\approx 11.34 \text{ g/cm}^3$) have proven exceptionally effective in attenuating gamma rays, particularly at low and intermediate energies where the Photoelectric Effect is dominant [6]. Despite its advantages, pure lead has drawbacks such as high toxicity and poor mechanical properties (low hardness and ductility). This has prompted researchers to develop lead-based alloys with other elements added to improve mechanical and thermal properties while maintaining or even enhancing their shielding capability [7]. To evaluate the effectiveness of shielding materials, it is essential to study fundamental physical parameters like the mass attenuation coefficient (MAC), cross-sections (molecular and electronic), effective atomic number (Z_{eff}), electron density, and mean free path (MFP). Computational codes —such as WinXCOM and Phy-X/PSD are used to study these parameters accurately and efficiently for both gamma ray and fast neutrons before the materials are fabricated and experimentally tested [8].

2. Materials and Methods

Calculation procedures

Despite the superior nuclear advantages of pure lead, it possesses certain drawbacks that limit its structural applications, such as its high toxicity and poor mechanical properties, including excessive ductility, low hardness, and weak creep resistance. To address these challenges, researchers are turning to the development of lead-based alloys by adding small quantities of other elements. This alloying process aims to improve the mechanical and thermal properties of lead while attempting to preserve, or even enhance, its outstanding shielding capability. Previous studies have shown that the addition of elements like copper (Cu) can strengthen and harden lead by forming a dispersed secondary phase within the lead matrix, which impedes dislocation movement. Similarly, the addition of elements like tellurium (Te) in trace amounts (up to 0.1%) has proven effective in significantly improving lead's resistance to creep and fatigue, in addition to increasing its corrosion resistance in certain environments. The selection of these alloying elements and their proportions plays a crucial role in achieving the desired balance between enhanced mechanical performance and high radiation shielding effectiveness [9-10].

Gamma-Ray Attenuation Parameters

The probability of interactions between incident photons and the target material is measured by the total mass attenuation coefficient (μ_t) (cm^2/g) [11,12].

$$\mu_t = \frac{\mu}{\rho} \quad (1)$$

Where the material density is indicated by ρ (g/cm^3) and the linear attenuation coefficient is represented by μ (cm^{-1}) [13]. The following formula is used to determine the total molecular cross-section $\sigma_{t.m}$ (barn/molecule) [14]:

$$\sigma_{t.m} = \mu_t \frac{M}{N_A} \quad (2)$$

Where N_A is Avogadro's number and M is the molecular weight [15]. The formula below is used to determine the total atomic cross-section ($\sigma_{t.a}$) (barn/atom) [16]:

$$\sigma_{t.a} = \frac{\sigma_{t.m}}{\sum_i n_i} \quad (3)$$

The following formula is used to determine the total electronic cross-section ($\sigma_{t.e}$) (barn/electron) [16]:

$$\sigma_{t.e} = \frac{1}{N_A} \sum_i f_i \frac{A_i}{Z_i} (\mu_t)_i \quad (4)$$

Each element's weight fraction in the compound is denoted by f_i . By using the following formula, the effective atomic number (Z_{eff}) is determined [17,18]:

$$Z_{eff} = \frac{\sigma_{t.a}}{\sigma_{t.e}} \quad (5)$$

The following formula is used to determine the electron density (N_{ele}) [19]:

$$N_{ele} = \frac{\mu_{t.m}}{\sigma_{t.e}} \quad (6)$$

The following equation is used to get the mean free path (λ) (cm) [20]:

$$\lambda = \frac{1}{\mu_t} \quad (7)$$

The Applied Shielding Materials

In the current employed calculations, a group of five lead-based alloys named S1, S2, S3, S4, and S5, were investigated to evaluate their gamma-ray shielding properties. The alloys were designed to have lead (Pb) as the primary constituent, with minor additions of copper (Cu) and tellurium (Te) as doping elements. The precise weight fraction (%) of each element in the samples was defined to systematically study the effect of trace compositional variations on the overall shielding efficiency. The elemental composition of the five alloys is detailed in Table 1 below.

Table 1. Elemental weight fraction (%) of the investigated Pb-Cu-Te alloys.

SAMP.	Pb %	Cu%	Te %
S 1	99.90	0.06	0.04
S 2	99.89	0.06	0.05
S 3	99.93	0.03	0.04
S 4	99.86	0.10	0.04
S 5	99.87	0.03	0.10

The selection of these compositions allows for a focused analysis on how minor adjustments—specifically, the trade-off between the High-Z element (Pb) and the lower-Z

doping elements (Cu, Te)—influence the key shielding parameters of the alloys. As indicated in Table (2), natural gamma radiation sources were applied in the current calculations.

Table 2. Energies sources and their energies [21,22].

No.	Radioactive source	E (MeV)
1	^{241}Am	0.05953
2	^{133}Ba	0.08099
3	^{137}Cs	0.6617
4	^{60}Co	1.178
5		1.332

Table 3. The density and molecular mass of the alloys under study.

Sample	Density of Sample (g/cm ³)	Molecular Mass of Sample
S 1	11.33653	207.081968
S 2	11.33602	207.0740076
S 3	11.33725	207.1250638
S 4	11.33558	207.024506
S 5	11.334186	207.0773

3. Results and Discussion

Table 4 presents the total mass attenuation coefficient calculated using the XCOM, NGCal, and Py-MILBUF codes at the incident gamma-ray photon energies.

Table 4. The mass attenuation coefficients (MAC) in cm²/g for the investigated alloys, calculated at various gamma-ray energies.

SA.	MAC								
	0.05953 MeV			0.08099 MeV			0.6617 MeV		
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF
S 1	5.121	5.123	5.120	2.346	2.345	2.419	0.1102	0.111	0.1108
S 2	5.121	5.123	5.121	2.346	2.344	2.4187	0.1102	0.111	0.1107
S 3	5.122	5.124	5.122	2.346	2.346	2.420	0.1102	0.1111	0.111
S 4	5.119	5.121	5.121	2.345	2.345	2.4189	0.1101	0.111	0.1106
S 5	5.123	5.125	5.119	2.347	2.346	2.4185	0.1101	0.111	0.11
SA.	1.178 MeV			1.332 MeV					
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF			
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF			
S 1	0.06153	0.06179	0.0618	0.05615	0.05639	0.0561			
S 2	0.06153	0.06178	0.06178	0.05615	0.05638	0.05607			
S 3	0.06153	0.0618	0.0619	0.05615	0.0564	0.0562			
S 4	0.06153	0.06178	0.06179	0.05615	0.05637	0.05608			
S 5	0.06153	0.06178	0.0617	0.05615	0.05638	0.05600			

The results clearly shows , that the values (MAC) for the five lead-based alloys follows a strong inverse relationship with the incident gamma-ray energy. The MAC values are highest at low energies (0.05953 and 0.08099 MeV), where the Photoelectric Effect, a mechanism highly dependent on the atomic number (Z), is the dominant interaction. As the energy increases into the intermediate and high ranges (0.6617 to 1.332 MeV), the dominance shifts to Compton Scattering, which is less dependent on Z, due to a sharp and continuous to decrease in the MAC values. A comparative analysis of the samples reveals that subtle differences in their chemical composition are accurately noted in the MAC values; samples with a higher fraction of High-Z elements, such as S3 (highest content of Pb) and S5 (higher Te content), consistently exhibit slightly higher attenuation coefficients, confirming that the shielding capability is enhanced by increasing the effective atomic number of the composite. Regarding the computational tools, an excellent, near-perfect agreement was observed between the XCOM and NGCal results, suggesting they utilize the same reliable NIST database and computational algorithms. While Py-MILBUF showed acceptable agreement across most of the energy spectrum, it yielded noticeably higher values specifically at 0.08099 MeV. This contrast is likely attributable to the proximity of this energy to the K-edge of lead (0.088 MeV), where the program's interpolation method may differ from, and be less precise than, that used by XCOM and NGCal, warranting caution when interpreting its results near the absorption edges of the constituent elements. Table 5 presents the total molecular cross-section calculated using Equation (2) at the incident gamma-ray photon energies.

Table 5. total molecular cross-section ($\sigma_{t,m}$) for the investigated alloys, calculated at various gamma-ray energies.

SA.	$\sigma_{t,m}$ (Barn/Molecule)								
	0.05953 MeV			0.08099 MeV			0.6617 MeV		
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF
S 1	1760.988	1761.675	1760.644	806.7325	806.3886	831.8354	37.8951	38.1702	38.10143
S 2	1760.920	1761.608	1760.9199	806.7014	806.01371	831.70024	37.89365	38.16874	38.06558
S 3	1761.698	1762.386	1761.698	806.9005	806.9005	832.3526	37.90299	38.21255	38.17816
S 4	1759.811	1760.499	1760.499	806.1648	806.1648	831.5702	37.85021	38.15961	38.0221
S 5	1761.636	1762.323	1760.26	807.0582	806.7143	831.6447	37.85986	38.16935	37.8255
SA.	1.178 MeV			1.332 MeV					
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF			
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF			
S 1	21.15867	21.24808	21.25152	19.30862	19.39115	19.29143			
S 2	21.15786	21.24383	21.24383	19.30788	19.38697	19.28037			
S 3	21.16308	21.25595	21.29034	19.31264	19.39863	19.32984			
S 4	21.1528	21.23875	21.24219	19.30326	19.3789	19.2792			
S 5	21.1582	21.24416	21.21665	19.30819	19.38728	19.25661			

The total molecular cross-section ($\sigma_{t,m}$), presented in table 5, closely follows the previously observed trend, decreasing sharply with increasing incident photon energy. This reflects the reduced probability of interaction at the molecular level as the dominant mechanism shifts from the high-probability Photoelectric Effect at low energies to the lower-probability Compton Scattering at higher energies. The subtle differences between the samples become more pronounced with this parameter, directly reflecting the influence of chemical composition and effective molecular weight. Sample S4, containing

the highest fraction of copper (the lightest element) and thus the lowest effective molecular weight, consistently exhibits the lowest molecular cross-section values. Conversely, sample S3, with the highest fraction of lead (the heaviest element) and the highest effective molecular weight, records the highest values. This confirms that the probability of a photon interacting with an average "molecule" increases with the molecule's weight. The excellent agreement between the XCOM and NGCal codes persists, reinforcing the data's reliability, while the notable discrepancy in the Py-MILBUF results at 0.08099 MeV remains evident, reaffirming that this deviation results from the database program's calculation dependent especially near the K-edge of lead. Table (6) presents the total electronic cross-section calculated using Equation (4) at the incident gamma-ray photon energies.

Table 6. total electronic cross-section (σ_{ele}) for the investigated alloys, calculated at various gamma-ray energies.

SA.	σ_{ele} (Barn/Electron)								
	0.05953 MeV			0.08099 MeV			0.6617 MeV		
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF
S 1	21.4857	21.4941	21.4815	9.8429	9.8387	10.1492	0.46236	0.4657	0.46487
S 2	21.4857	21.4940	21.4857	9.8429	9.8345	10.1479	0.46236	0.4657	0.4645
S 3	21.4908	21.4992	21.4908	9.8433	9.8433	10.1538	0.46237	0.4662	0.4657
S 4	21.4762	21.4846	21.4846	9.8382	9.8382	10.14823	0.4619	0.4657	0.4640
S 5	21.4946	21.5030	21.4778	9.84733	9.8431	10.1473	0.46195	0.4657	0.46153
SA.	1.178 MeV			1.332 MeV					
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF			
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF			
S 1	0.258156	0.259247	0.259289	0.235584	0.236591	0.235374			
S 2	0.258155	0.259204	0.259204	0.235583	0.236548	0.235247			
S 3	0.258166	0.259299	0.259719	0.235593	0.236642	0.235803			
S 4	0.258142	0.259191	0.259233	0.235571	0.236494	0.235277			
S 5	0.258162	0.259211	0.258875	0.235589	0.236554	0.23496			

The total electronic cross-section (σ_{ele}), presented in Table (6), follows the general trend of the previous parameters, decreasing sharply with increasing photon energy, which reflects the reduced interaction probability per electron at higher energies. This parameter reveals a fundamental physical insight when analyzing the effect of chemical composition. In the intermediate and high-energy regions (0.6617 MeV and above), where Compton Scattering is dominant, the σ_{ele} values for all five samples become nearly identical. This confirms the principle that the Compton interaction probability depends primarily on the electron density and is almost independent of the target atom. In contrast, at low energies (0.05953 and 0.08099 MeV), where the Photoelectric Effect prevails, small but significant differences persist. The strong dependence of this phenomenon on the atomic number (proportional to Z^4) is not entirely canceled out by dividing by Z_{eff} , resulting in samples with a higher effective atomic number (like S3) exhibiting a slightly larger electronic cross-section. Regarding the software comparison, the near-perfect agreement between XCOM and NGCal continues, while the notable discrepancy in the Py-MILBUF results at 0.08099 MeV remains, confirming that this deviation originates from the calculation of the fundamental attenuation coefficient near the absorption edge of lead. Table 7 presents the Mean Free Path calculated using Equation (7) at the incident gamma-ray photon energies.

Table 7. Mean free path (MFP) for the investigated alloys, calculated at various gamma-ray energies.

SA.	MFP (cm)								
	0.05953 MeV			0.08099 MeV			0.6617 MeV		
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF
S 1	0.017225	0.017219	0.017229	0.0376	0.037616	0.036466	0.800457	0.794688	0.796123
S 2	0.017226	0.017219	0.017226	0.037602	0.037634	0.036472	0.800493	0.794724	0.796878
S 3	0.017221	0.017214	0.017221	0.037598	0.037598	0.036448	0.800407	0.793923	0.794638
S 4	0.017236	0.017229	0.017229	0.037624	0.037624	0.036475	0.80135	0.794852	0.797727
S 5	0.017222	0.017215	0.017236	0.037592	0.037608	0.036481	0.80135	0.794852	0.802078
SA.	1.178 MeV			1.332 MeV					
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF			
	XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF			
S 1	1.4336	1.4276	1.42735	1.57098	1.56429	1.57238			
S 2	1.43368	1.4279	1.42788	1.5710	1.5646	1.5733			
S 3	1.4335	1.42726	1.4249	1.5709	1.5639	1.56948			
S 4	1.4339	1.42811	1.42788	1.5713	1.5652	1.5733			
S 5	1.4339	1.4281	1.42996	1.5713	1.5649	1.5755			

The results demonstrate a clear and strong direct relationship between the mean free path (MFP) and photon energy, with MFP values increasing substantially at higher energies. This indicates that high-energy photons are more penetrating and require a greater material thickness for attenuation, reflecting their lower interaction probability at high energies (dominated by Compton Scattering) compared to low energies (dominated by the Photoelectric Effect). When comparing the different samples, compositional variations translate into distinct differences in shielding capability. Sample S3, containing the highest fraction of lead, consistently exhibits the shortest MFP across all energies, confirming it as the most effective radiation attenuator among the five alloys. Conversely, sample S4, with the lowest lead content, shows the longest MFP, rendering it the least effective shield. Regarding the software comparison, the excellent agreement between XCOM and NGCal persists. The notable discrepancy in the Py-MILBUF results at 0.08099 MeV remains, where it calculates a distinctly lower MFP value, directly reflecting its divergent calculation of the attenuation coefficient at this energy near the K-edge of lead. Table 8 presents the effective atomic number (Z_{eff}) and electron density (N_{ele}) values, which were calculated using Equations (5) and (6), respectively.

Table 8. The effective atomic number (Z_{eff}) and electron density (N_{ele}) for the investigated alloys.

Z_{eff}			$N_{\text{ele}} \times 10^{24}$ (electron/g)		
XCOM	NGCal	Py-MILBUF	XCOM	NGCal	Py-MILBUF
81.96076	81.96076	81.96076	0.238344	0.238344	0.238344
81.95786	81.95786	81.95786	0.238345	0.238345	0.238345
81.97458	81.97458	81.97458	0.238335	0.238335	0.238335

81.94239	81.94239	81.94239	0.238357	0.238357	0.238357
81.95706	81.95706	81.95706	0.238339	0.238339	0.238339

The results clearly show that the effective atomic number (Z_{eff}) values for all samples are very close to the atomic number of lead ($Z=82$), as expected, given that lead constitutes over 99.8% of each alloy's composition. The subtle yet significant differences in Z_{eff} values directly reflect their chemical makeup: sample S3, with the highest lead fraction (99.93%), possesses the highest Z_{eff} (81.974), making it the most effective for Z-dependent interactions like the Photoelectric Effect. Conversely, sample S4, with the lowest lead and highest copper content, has the lowest Z_{eff} (81.942), slightly reducing its effectiveness. The electron density (N_{ele}) is constant for each sample and does not vary with energy, showing very similar values across all alloys (approximately 0.238×10^{24} electrons/g). This indicates that the number of electrons per unit mass is not significantly altered by these minor compositional changes, a crucial factor in the Compton Scattering dominant region. A key observation from these results is the perfect agreement among the three codes (XCOM, NRCAL, and Py-MILBUF), confirming that the calculation of Z_{eff} and N_{ele} relies on direct equations using chemical composition as the primary input, leaving no room for the energy-dependent discrepancies previously noted in the attenuation coefficient calculations.

4. Conclusion

The results from the three programs showed excellent agreement, confirming the reliability of the calculated data for parameters such as the mass attenuation coefficient (MAC), effective atomic number (Z_{eff}), and mean free path (MFP). A strong dependence on both photon energy and chemical composition was observed, with all attenuation parameters decreasing at higher energies, consistent with the transition from the Photoelectric Effect to Compton Scattering as the dominant interaction mechanism. It was conclusively determined that the alloy S3, possessing the highest weight fraction of lead (99.93%), exhibited superior shielding performance across the entire energy range, evidenced by the highest MAC and Z_{eff} values and the shortest MFP. Conversely, the S4 alloy, with the lowest lead content, was the least effective shield. This work confirms that even minor variations in the concentration of the high-Z element significantly influence the shielding capability of lead-based alloys, providing a valuable theoretical basis for the design and optimization of advanced radiation shielding materials.

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