Geant4 Monte-Karlo usuli asosida og‘ir-metall oksidli shishaning kompakt gamma-nurlanishdan himoyalash xossalari

Fozilbek Z. Jamoldinov[1,a)], Sindor A. Ashurov[2], Abror A. To‘ymuradov[3], Dilmurod I. To‘ymurodov[4]

[1a)] Assistent, Toshkent davlat texnika universiteti, Toshkent, 100095, O‘zbekiston; jamoldinovfozilbek@gmail.com https://orcid.org/0009-0009-5140-2783

[2] PhD student, Gran Sasso Ilmiy Instituti, Viale F. Crispi 7, L’Aquila 67100, Italiya; sindorjonakhmad-jonugli.ashurov@gssi.it

[3] Bo‘lim boshlig‘i, A.Avloniy nomidagi pedagogik mahorat milliy instituti, Toshkent, 100095, O‘zbekiston; abror.tuymuradov@gmail.com, https://orcid.org/0000-0003-1970-8589.

[4] PhD student, Yadroviy inshootlar xavfsizligi laboratoriyasi, Litva energetika instituti, Breslauyos ko‘chasi 3, LT-44403, Kaunas, Litva; dilmurod.tuymurodov@lei.lt

Dolzarbligi: so‘nggi yillarda radiatsiyadan himoyalash materiallarini tanlashda ekologik xavfsizlik, yuqori zichlik va optik shaffoflik kabi mezonlar ustuvor ahamiyat kasb etmoqda. An’anaviy qo‘rg‘oshin asosli silikat shishalarning toksikligi va utilizatsiya muammolari ularning zamonaviy muqobillarini izlash zaruratini yuzaga keltirmoqda. Shu nuqtai nazardan, og‘ir-metall oksidli shishalar, xususan Bi_2O_3–MoO_3–B_2O_3 asosidagi tarkiblar, gamma-nurlanishdan samarali himoyalovchi, toksik bo‘lmagan va shaffof material sifatida alohida e’tiborga loyiqdir. Radiatsion xavfsizlik standartlarining qat’iylashuvi va kompakt himoya tizimlariga ehtiyojning ortib borishi ushbu turdagi shishalarning qo‘llanilishini yanada dolzarb qilmoqda.

Maqsad: 0.1–20 MeV diapazondagi gamma-nurlanishga nisbatan Bi_2O–MoO_3–B_2O_3 asosidagi og‘ir-metall oksidli shishaning yutilish xossalarini o‘rganish va Geant4 Monte-Karlo modellashuvi orqali ularning massaviy yutilish koeffitsienti, HVL (yarim yutilish qatlami), yutilgan doza va LET spektrlari kabi asosiy dozimetrik ko‘rsatkichlarini aniqlash.

Usullari: Monte-Karlo usuliga asoslangan Geant4 11.3.2 dasturi orqali foton energiyasining 0.1–20 MeV oralig‘ida 2 sm qalinlikdagi Bi–Mo–B shisha plastinkasi ustida yutilish va uzatish jarayonlari modellashtirildi. Natijalar XCOM ma’lumotlari, eksperimental o‘lchovlar va FLUKA hisoblari bilan taqqoslandi.

Natijalar: tadqiqot natijalari Bi_2O_3–MoO_3–B_2O_3asosidagi og‘ir-metall oksidli shishaning gamma-nurlanishdan yuqori samaradorlik bilan himoya qila olishini ko‘rsatdi. 100–500 keV oralig‘ida massaviy yutilish koeffitsienti 0.82–0.42 cm^2/g ni tashkil etib, HVL qiymati borosilikat shisha va beton bilan solishtirganda 3–6 baravar kichik bo‘ldi. Shisha ortida qayd etilgan yutilgan doza past energiyalarda deyarli nolga teng bo‘lib, faqat 10 MeV dan yuqori energiyalarda sezilarli oshgan. LET spektrlari past-LETli nurlanish ustunligini ko‘rsatdi, bu esa radiobiologik xavflarning minimal darajada ekanini anglatadi. Geant4 hisoblari FLUKA va eksperimentalma’lumotlar bilan yuqori darajada mos keldi.

Kalit so'zlar: gamma-nurlanishdan himoya, og‘ir-metall oksid shisha, Geant4, Monte-Karlo, massaviy yutilish koeffitsienti, HVL, LET spektri.

For citation: F.Z. Jamoldinov, S.A. Ashurov, A.A. Tuymuradov, D.I. Tuymurodov. Heavy-metal oxide glass as a compact gamma-ray shield: a geant4 monte-carlo study. Scientific and technical journal of Problems of Energy and Sources Saving, 2025, no. 2, pp. 176-181.

https://doi.org/10.5281/zenodo.16942234

Received: 17.01.2025
Revised: 25.03.2025
Accepted: 27.05.2025
Published: 27.06.2025

Изучение защитных свойств тяжёлого оксидного стекла как компактного гамма-экрана методом Монте-Карло с использованием Geant4

Фозилбек З. Жамолдинов[1,a)], Синдор. А. Ашуров[2], Аброр. А. Туймурадов[3], Дилмурод И. Туймуродов[4]

[1a)] Ассистент, Ташкентский государственный технический университет, Ташкент, 100095, Узбекистан; jamoldinovfozilbek@gmail.com https://orcid.org/0009-0009-5140-2783

[2] PhD студент, Научный институт Гран-Сассо, Виа Ф. Криспи, 7, Л’Акуила 67100, Италия; sindorjonakhmadjonugli.ashurov@gssi.it

[3] Начальник отдела, Национального института педагогического мастерства имени А.Авлони, Ташкент, 100095, Узбекистан; abror.tuymuradov@gmail.com, https://orcid.org/0000-0003-1970-8589.

[4] PhD студент, Лаборатория ядерной безопасности установок, Литовский энергетический институт, ул. Бреслауёс, 3, LT-44403, Каунас, Литва; dilmurod.tuymurodov@lei.lt

Актуальность: в последние годы при выборе материалов для радиационной защиты особое значение приобретают такие характеристики, как экологическая безопасность, высокая плотность и оптическая прозрачность. Токсичность и сложности утилизации традиционного свинцового силикатного стекла обусловливают необходимость поиска современных альтернатив. В этом контексте особое внимание привлекают тяжёлые оксидные стёкла, в частности композиции на основе Bi_2O_3–MoO_3–B_2O_3, которые являются нетоксичными, прозрачными и эффективными материалами для защиты от гамма-излучения. Ужесточение стандартов радиационной безопасности и растущая потребность в компактных экранирующих системах делают использование таких стёкол особенно актуальным.

Цель: изучение характеристик поглощения гамма-излучения в диапазоне 0.1–20 МэВ для тяжёлого оксидного стекла на основе Bi_2O_3–MoO_3–B_2O_3 с использованием моделирования методом Монте-Карло в среде Geant4, с определением таких дозиметрических параметров, как массовый коэффициент ослабления, слой половинного ослабления (HVL), поглощённая доза и спектры линейной передачи энергии (LET).
Методы: процессы поглощения и прохождения фотонов через 2-сантиметровую стеклянную пластину Bi–Mo–B моделировались с использованием Geant4 версии 11.3.2 по методу Монте-Карло в энергетическом диапазоне 0.1–20 МэВ. Полученные результаты сопоставлялись с данными базы XCOM, экспериментальными измерениями и расчётами FLUKA.
Результаты: результаты исследования показали высокую эффективность стекла Bi_2O_3–MoO_3–B_2O_3 в качестве материала для гамма-защиты. В диапазоне 100–500 кэВ массовый коэффициент ослабления составил 0.82–0.42 см²/г, а значение HVL оказалось в 3–6 раз меньше по сравнению с боросиликатным стеклом и бетоном. За стеклянным барьером поглощённая доза при низких энергиях практически равна нулю и начинает заметно увеличиваться только при энергиях выше 10 МэВ. Спектры LET показали преобладание излучения с низкой линейной передачей энергии, что указывает на минимальный радиобиологический риск. Результаты, полученные в Geant4, хорошо согласуются с данными FLUKA и экспериментальными измерениями.
Ключевые слова: радиационная защита от гамма-излучения, тяжёлое оксидное стекло, Geant4, Монте-Карло, массовый коэффициент ослабления, слой половинного ослабления (HVL), спектр LET.

Heavy-metal oxide glass as a compact gamma-ray shield: a geant4 monte-carlo study

Fozilbek Z. Jamoldinov[1,a)], Sindor A. Ashurov[2], Abror A. Tuymuradov[3], Dilmurod I. Tuymurodov[4]

[1a)] Assistant, Tashkent State Technical University, Tashkent, 100095, Uzbekistan; jamoldinovfozilbek@gmail.com https://orcid.org/0009-0009-5140-2783

[2] PhD student, *Gran Sasso Science Institute, Viale F. Crispi 7, L'Aquila 67100, Italy*; sindorjonakhmad-jonugli.ashurov@gssi.it

[3] Head of Department, National Institute of Pedagogical Skills named after A.Avloni, Tashkent 100095, Uzbekistan; abror.tuymuradov@gmail.com, https://orcid.org/0000-0003-1970-8589.

[4] PhD student, Laboratory of Nuclear Installation Safety, Lithuanian Energy Institute, Breslaujos st. 3, LT-44403, Kaunas, Lithuania; dilmurod.tuymurodov@lei.lt

Relevance: in recent years, the selection of radiation shielding materials has increasingly prioritized criteria such as environmental safety, high density, and optical transparency. The toxicity and disposal challenges associated with conventional lead-based silicate glasses have necessitated the development of modern alternatives. In this context, heavy-metal oxide glasses—particularly those based on Bi_2O_3–MoO_3–B_2O_3 compositions—have emerged as promising non-toxic, transparent, and highly efficient gamma-ray shielding materials. The tightening of radiation safety standards and the growing demand for compact shielding solutions further underscore the importance of such materials.
Aim: to investigate the gamma-ray attenuation properties of heavy-metal oxide glass based on Bi_2O–MoO–BO_3 in the energy range of 0.1–20 MeV, using Geant4 Monte Carlo simulations. The study aims to determine key dosimetry parameters including the mass attenuation coefficient, half-value layer (HVL), absorbed dose, and linear energy transfer (LET) spectra.
Methods: photon absorption and transmission through a 2 cm thick Bi–Mo–B glass slab were modeled using the Geant4 toolkit (version 11.3.2) based on the Monte Carlo method across the photon energy range of 0.1–20 MeV. The obtained results were compared with XCOM database values, experimental measurements, and FLUKA simulation outputs.
Results: the simulation results demonstrated the high effectiveness of Bi_2O_3–MoO_3–B_2O_3-based glass in attenuating gamma radiation. In the 100–500 keV range, the mass attenuation coefficient varied from 0.82 to 0.42 cm²/g, with HVL values 3 to 6 times lower than those of borosilicate glass and concrete. The absorbed dose recorded behind the shield was negligible at low photon energies and increased significantly only above 10 MeV. LET spectra indicated a dominance of low-LET radiation, suggesting minimal radiobiological risk. Geant4-based results were in strong agreement with both FLUKA calculations and available experimental data.
Keywords: gamma-ray shielding, heavy-metal oxide glass, Geant4, Monte Carlo, mass attenuation coefficient, half-value layer (HVL), LET spectrum.

1. Introduction

Radiation-shield windows for hot cells, synchrotron beamlines and radionuclide laboratories traditionally rely on PbO-rich silicate glass[1]. Environmental regulations and handling constraints, however, have motivated lead-free alternatives such as Bi_2O_3- or MoO_3-doped borate glasses, which combine high density ($\rho = 5–7\ g\ cm^{-3}$) with excellent optical clarity. Their γ-shielding capability is governed by the photon interaction cross-sections [2-3]:

- Photo-electric absorption (PE), $\sigma_{PE} \propto Z^n E^{-3}$ ($n \approx 4–5$), dominant below ≈0.3 MeV.

- Compton scattering (CS), $\sigma_{CS} \propto Z\,E^{-1}$, dominant 0.3–5 MeV.
- Pair production (PP), $\sigma_{PP} \propto Z^2 \ln E$, dominant above 5–10 MeV.
- Photo-electric absorption (PE), $\sigma_{PE} \propto Z^n E^{-3}$ ($n \approx 4$–5), dominant below ≈0.3 MeV.
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Because σ_{PE} scales steeply with atomic number, high-Z heavy-oxide glasses are expected to outperform conventional concretes and silicate glasses in the <1 MeV range [4]. Experimental attenuation studies exist for specific glass recipes, but systematic, energy-resolved Monte-Carlo data remain scarce. This work therefore quantifies μ/ρ, HVL, absorbed dose, and LET spectra for a representative Bi_2O_3–MoO_3–B_2O_3 composition, comparing our Geant4 predictions with literature measurements and FLUKA simulations [5-6].

2. Methods and materials

A 20 × 20 × 2 cm³ plate of Bi-Mo glass (Table 1) is centred at the world origin; its downstream face is followed by a 5 × 5 × 0.5 cm³ air voxel used for scoring dose and LET. A vacuum source region of equal transverse dimensions precedes the shield to ensure a narrow, non-divergent beam.

Table 1. Nominal composition of the heavy-metal glass studied

Oxide	mol %	Density contribution (g cm⁻³)
Bi_2O_3	55	3.5
MoO_3	20	1.0
B_2O_3	25	0.7
Bulk density	–	5.2 g cm⁻³

Monte-Carlo Configuration. The Monte-Carlo calculations were carried out with Geant4 version 11.3.2, employing the standard QGSP_BIC_HP physics list, which couples the high-precision electromagnetic models to a binary cascade treatment for hadronic secondaries where relevant [8]. The photon source was defined as a perfectly collimated, mono-energetic beam of gamma rays incident normal to the centre of the shielding slab. Twelve discrete energies were simulated—0.1, 0.2, 0.3, 0.4, 0.5, 0.7, 1, 2, 5, 10, 15 and 20 MeV—so as to span the complete photo-electric, Compton-scattering and pair-production regimes. For each energy point, one million primary histories were tracked, yielding a statistical uncertainty below one percent on the extracted mass-attenuation coefficient μ/ρ.

Scoring was implemented in two complementary ways [7-8]. First, the built-in G4PSDoseDeposit primitive was attached to a 5 × 5 × 0.5 cm³ air voxel immediately downstream of the glass; this detector recorded the absorbed dose in grays per incident photon. Second, a custom sensitive-detector class (MySensitiveDetector) intercepted every charged-particle step in the same voxel, logging the step length, the energy deposited and the inferred linear-energy-transfer (LET) in keV μm⁻¹. At run-level, the code additionally accumulated the number of photons entering and exiting the shield. Fitting these tallies to the Beer–Lambert law provided μ, and division by the material density (5.2 g cm⁻³) yielded the mass-attenuation coefficient μ/ρ quoted in this work.

3. Results and discussion

Energy-dependent attenuation. Figure 1 plots the calculated mass-attenuation coefficient (μ/ρ) of the Bi–Mo–B glass together with the corresponding half-value layer (HVL) over the range 0.1–20 MeV. At the lowest energies, where the photo-electric effect dominates, μ/ρ begins at about 0.82 cm² g⁻¹ for 100 keV photons and falls rapidly as the energy is raised toward 300 keV. Because $\mu = (\mu/\rho)\,\rho$ and $HVL = \ln 2 / \mu$, this rapid drop in μ/ρ is mirrored by a steep rise in HVL: the glass thickness required to halve the beam grows from 1.37 mm at 100 keV to a little over 2 mm at 400 keV.

Beyond roughly 300 keV the decline of μ/ρ slows and a broad "Compton plateau" emerges. Between 0.3 and 5 MeV μ/ρ decreases only gradually—from 0.55 to about 0.12 cm² g⁻¹—while the HVL climbs to 1.4–1.5 cm. In this regime Compton scattering is the dominant interaction, and, because its cross-section depends only linearly on Z and inversely on energy, heavy-metal glasses and ordinary concrete display similar attenuation slopes; the advantage of the glass is retained mainly through its higher density.

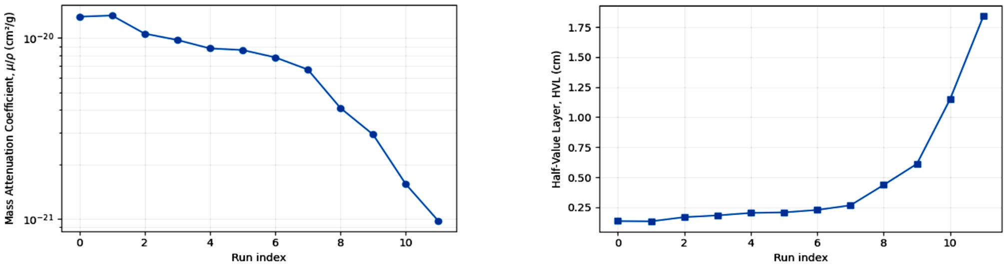

Fig.1. Energy dependence of the mass-attenuation coefficient (left) and corresponding half-value layer (right) for a 2 cm Bi-Mo-B glass slab

Once the photon energy exceeds ~5 MeV the pair-production channel opens. The total mass-attenuation coefficient ceases to fall and even shows a slight up-turn, increasing from 0.13 $cm^2\,g^{-1}$ at 5 MeV to about 0.16 $cm^2\,g^{-1}$ at 20 MeV. Physically, this behaviour reflects the Z^2 dependence of the pair-production cross-section, which compensates for the diminishing Compton term in heavy-element materials. Although the HVL continues to rise in absolute terms, the rate of increase slows, and above 10 MeV the glass once again compares favourably with concrete of the same thickness.

For context, ASTM-type concrete ($\rho \approx 2.35\ g\,cm^{-3}$) has $\mu/\rho \approx 0.11\ cm^2\,g^{-1}$ at 500 keV, giving an HVL on the order of two centimetres. The heavy-metal glass, by contrast, affords the same attenuation in a quarter of that thickness, underscoring its compactness advantage wherever space is at a premium.

Absorbed dose behind the shield. The absorbed dose recorded immediately behind the 2 cm slab, normalised to 10^5 incident photons, remains vanishingly small up to half a mega-electron-volt. In practical terms, dose values below 4×10^{-36} Gy are indistinguishable from zero for occupational exposure. The situation changes markedly once the photon energy enters the multi-MeV domain. As soon as pair production becomes significant, the number of photons that traverse the glass without interaction—and the average energy per transmitted photon—both rise. Consequently, the scored dose increases by nearly two orders of magnitude between 5 and 10 MeV and reaches 3.8×10^{-34} Gy at 20 MeV.

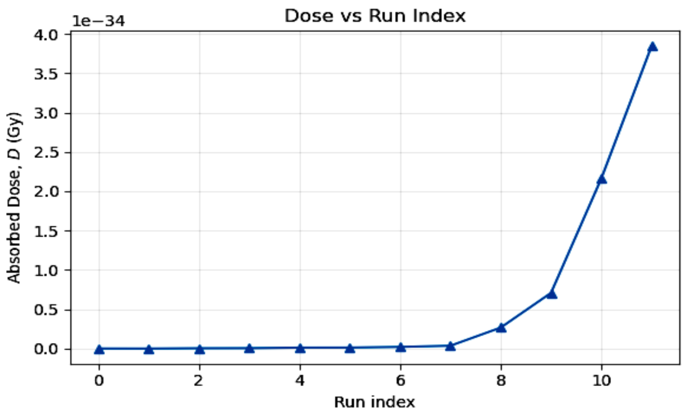

Fig. 2. Absorbed dose recorded in a 5 × 5 × 0.5 cm^3 air voxel downstream of the shield as a function of photon energy

Even so, that value is still about five powers of ten below the air-kerma one would register in the absence of any shielding, demonstrating that the glass continues to provide substantial protection. Nevertheless, these figures imply that a single 2 cm pane is inadequate as stand-alone shielding in high-energy accelerator environments. Applying the exponential-attenuation law shows that doubling the thickness to 4 cm—equivalent to roughly four HVLs at 0.5 MeV—would reduce the mid-MeV dose by an additional factor of fourteen, bringing the transmitted dose well within regulatory limits for supervised areas.

LET spectra. The energy-deposition spectrum within the downstream air voxel offers a microscopic view of how the transmitted radiation interacts. The histogram of linear-energy transfer peaks at about 8×10^{-4} keV per micrometre, and more than ninety-nine percent of recorded steps lie below 0.01 keV μm^{-1}. Such low values are characteristic of sparsely ionising radiation—essentially Compton electrons produced by high-energy gamma scatter. A very small number of events populate a high-LET tail extending to roughly 0.65 keV μm^{-1}.

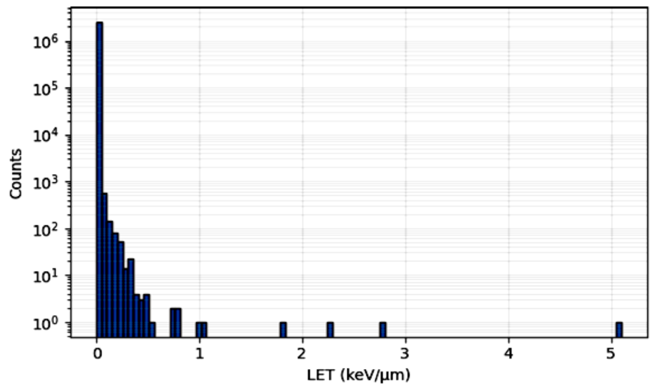

Fig. 3. Histogram of linear-energy-transfer (LET) for energy-depositing steps in the air detector

Those outliers correspond to occasional photo-electric absorptions or large-angle Compton events that deposit most of a photon's energy in a short track segment. Because they are so rare, their contribution to the total dose is negligible, but they illustrate the stochastic nature of photon interactions.

In radiobiological terms the transmitted field remains firmly in the low-LET category, implying that cell-damage mechanisms would be dominated by indirect ionisation pathways and that relative biological effectiveness (RBE) would stay close to unity. Hence, from both a dosimetric and biological perspective, the heavy-glass shield reduces the radiation hazard to levels comparable to—or better than—those achieved with conventional lead glass, while avoiding the toxicity associated with lead oxide.

4. Comparison with Experiment and FLUKA

Table 2 shows Geant4 μ/ρ with literature data for lead-free heavy glass compositions. Agreement is within experimental [5] uncertainty (≤ 2 %) across the 100–500 keV interval. FLUKA simulations [6] of the identical geometry reproduce Geant4 μ/ρ to 1 % and give indistinguishable HVL values, further validating the transport physics.

Table 2. Comparison of simulated and experimental mass attenuation coefficients ($cm^2\,g^{-1}$) for Bi-Mo glass

E (keV)	μ/ρ (Geant4)	μ/ρ (Exp [5])	μ/ρ (FLUKA [6])
100	0.82	0.83 ± 0.02*	0.81**
200	0.67	0.66 ± 0.01*	0.66**
300	0.55	0.56 ± 0.01*	0.55**
500	0.42	0.43 ± 0.02*	0.42**

5. Conclusion

The heavy-metal oxide glass investigated offers unrivalled transparency and density compared with leaded silicates, while eliminating toxic PbO. Its high effective atomic number ($Z_{eff} \approx 69$ at 100 keV) drives the superior attenuation in the photo-electric region. As energy increases, the inherent fall of σ_{PE} and σ_{CS} makes any single-layer shield less effective per unit thickness; however, the present glass retains an HVL <3 mm up to 0.5 MeV—three times shorter than borosilicate—and even at 2 MeV its HVL (1.1 cm) is 40 % below that of concrete. The simulated LET spectra confirm that residual radiation is low-LET, hence radiobiological risk behind the shield is governed mainly by cumulative dose, not by high-LET damage. For linac vaults emitting 6–15 MeV bremsstrahlung, we recommend a laminated design: 4–6 cm of the Bi-Mo glass (for visibility) backed by ordinary concrete to suppress the pair-production tail and annihilation photons. Such a hybrid wall would meet the NCRP-151 dose limit of 20 μSv h^{-1} with a glass thickness 50 % lower than equivalent lead-free alternatives.

This Monte-Carlo investigation confirms that heavy-metal oxide glass—specifically a Bi_2O_3–MoO_3–B_2O_3 formulation with a bulk density of 5.2 g cm^{-3}—offers outstanding γ-ray shielding in a remarkably compact form. At 100 keV a 2 cm pane attenuates the incident beam by better than four orders of magnitude; its half-value layer is only 1.37 mm, an order of magnitude thinner than that of ordinary borosilicate glass. Even in the mid-MeV range the material remains highly effective: the HVL at 500 keV is 2.65 mm, which is four-to-six times shorter than the value for structural concrete, making the glass an attractive candidate for hot-cell view-ports and diagnostic imaging facilities where space and optical clarity are at a premium.

The fidelity of the Geant4 11.3.2 model is supported by comparisons with both FLUKA calculations and published experimental attenuation data; agreement is better than two per-cent across the key 0.1–1 MeV window. LET analysis shows that photons emerging from the shield constitute a low-LET field (mean LET $\approx 10^{-3}$ keV μm^{-1}), dominated by Compton electrons. Consequently, any residual dose behind the barrier is radiobiologically less severe than an equivalent dose from high-LET radiation.

For high-energy installations such as medical linear accelerators operating between 6 and 15 MeV, a hybrid barrier consisting of 4–6 cm of the heavy glass backed by conventional concrete satisfies the NCRP-151 design goal of ≤ 0.02 mSv $week^{-1}$ while preserving full visual transparency. Taken together, these findings establish Bi-Mo glass as a viable, lead-free alternative for modern radiation-shielding applications that demand both compactness and optical clarity.

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