Supplementary Information (SI) for Materials Advances. This journal is © The Royal Society of Chemistry 2025

S. MATERIALS AND METHODS: Theoretical and computational background

1. Web-Based Software

S.1 XCOM program

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The XCOM software [1-4] is the oldest used web-based program to calculate the radiation mass attenuation coefficients of defined samples. XCOM program is a user friendly calculation program and the input parameter specifications are quite flexible and easy to access via internet database. In the XCOM program, each sample (*i.e.*, shielding material) was defined by their elemental fractions. The mass attenuation coefficient of the investigated materials is then calculated by the XCOM program. This program does not perform the calculation of the other shielding parameters (*i.e.*, LAC) and have to be calculated separately depending on the user external software. Very recently, Web-based programs have emerged to overcome these difficulties making it easy for the scientists to perform all of the shielding parameters via online platform [4].

S.2 Phys-X/SPD Software

A user friendly online Photon Shielding and Dosimetry (PSD) software available at https://phy-x.net/PSD has been developed for calculation of parameters relevant to shielding and Dosimetry [4]. These parameters include linear and mass attenuation coefficients (LAC, MAC), half and tenth value layers (HVL, TVL), mean free path (MFP), effective atomic number and electron density (Z_{eff}, N_{eff}), and exposure buildup factors (EABF, EBF). The software can generate data on shielding parameters in the continuous energy region (1 keV-15 MeV). The software is freely available online after having register into the Phy-X platform [4].

S.3 shielding parameters basic relations

When a material of a thickness 'x' is placed in the way of a radiant X-ray or gamma beam, the intensity of this beam is attenuated according to the exponential attenuation law (Beer Lambert's law)

$$\frac{I}{I_0} = e^{-\mu x} \tag{13}$$

where I_0 and I are the intensity before and after the attenuation respectively, x is sample thickness and μ is the linear attenuation coefficient (LAC, μ in cm⁻¹) [5]. The mass attenuation coefficient (MAC in cm²/g) is a quantity that evaluates the probability of interaction of the photon with the material. MAC can be theoretically evaluated according to the mixture rule [4]

$$MAC = \mu_m = \frac{\mu}{\rho} = \frac{1}{x} \ln(\frac{I_0}{I})$$
 (14)

The MAC values have been calculated using the above mentioned web-based programs. The difference (Diff %) between the two calculated MAC values is evaluated according to the following equation

$$Diff(\%) = \frac{\left| (\mu_m)_{Phys} - (\mu_m)_{BUF} \right|}{(\mu_m)_{Phys}} \tag{15}$$

However, the HVT is shielding parameter that introduces the thickness of the shielding material that is able to diminish the incoming photon intensity to half of its value and can be calculated based on the LAC values according to the following equation [5]

$$HVL = \frac{\ln(2)}{\mu} \tag{16}$$

The transmission factor (TF) is used to predict the ratio of γ -photon flux that can transmit a known thickness at any gamma photon energy and can be calculated as:

$$TF(\%) = \frac{I_0}{I} = e^{-\mu x}$$
 (17)

Also, the radiation protection effectiveness (RPE) is defined as:

$$RPE=1-TF (18)$$

Another important shielding property which may be derived from the basic physical quantities presented above is the removal cross-section (Σ_R) which is defined as: the probability of a neutron collision in a specific homogenous material. The effective removal cross-section of the current glasses can be calculated based on the value of $\Sigma_{R/\rho}$ for each element that is used to prepare the glass mixture [5]:

$$\sum_{R/\rho} = \sum_{i} w_{i} \left(\sum_{R/\rho} \right)_{i} \quad \text{and} \quad$$

$$\sum_{R} = \sum_{i} \rho_{i} \left(\sum_{R/\rho} \right)_{i} \tag{19}$$

where, ρ_i is the partial density of each element in the glass sample (g.cm⁻³), ρ is the total sample density (g.cm⁻³). In the current study, the effective removal cross-section was also determined using the new friendly Phy-X/PSD program [5].

References

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