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Comparative Study of Micro and Nano Size WO_3/E44 Epoxy Composite as Gamma Radiation Shielding Using MCNP and Experiment

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The radiation shielding characteristics of 50 wt% WO_3/E44 epoxy composite in various gamma energies from 80 keV to 1.33 MeV are investigated via the MCNP code. Thus two scales are considered for WO_3 filler particles: micro and nano with sizes of 1 μm and 50 nm, respectively. The simulation results show that WO_3 nano particles exhibit a larger increase in linear attenuation coefficient in comparison with micro size particles. Finally, validation of simulation results with the published experimental data shows a good agreement.

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Polymer composites exhibit potential applications in industry and medical care,[1,2] gamma and neutron radiation shielding,[3–7] electromagnetic interference (EMI) devices,[8,9] and dosimeters.[10–18] High-Z elements may be unable to block all types of radiations, particularly the emissions of neutrons in space or nuclear laboratories, and also restricted in some applications due to the heavy weight, bulky space, and toxicity (lead).[19–21] Therefore, non-toxic 'lead-free' filler-reinforced polymer composite for its lightweight, workability, and ability to effectively attenuate radiation has aroused great public interest in many areas, especially in medical treatment, nuclear plant and mobile nuclear devices.[22] Epoxy matrix composite loaded with high concentrations of high-Z fillers has become an attractive candidate, for radiation shielding.[22] The effect of particle size of tungsten oxide in WO_3/epoxy composite at x-ray tube voltages of 25–120 kV has been investigated.[23] Polymer composites are light, low cost and easily processed,[10,11] thus these kinds of materials via mixing with high-Z materials in the particular weight fractions of the inclusions or fillers have potential applications as radiation shielding materials.

Some studies have been carried out on the effect of shielding materials grain size on linear attenuation coefficients.[22,24–26] It is widely believed that nano-sized particles are able to disperse more uniformly within the matrix with fewer agglomerations when compared with micro-sized particles, thus improving the radiation attenuation ability of the materials.

Nanostructured materials are defined as those materials whose structural elements have dimensions in the range of 1–100 nm.[27] These materials can be composed of nano-sized grains, which consist of many atoms.[28] Grains of conventional materials have sizes that are in the range of tens of microns to one or more millimeters.[28] Due to their very small sizes, these materials can present novel chemical and physical properties relative to the same chemical compound with dimensions in the microscopic or macroscopic range.[29] Nano materials can also exhibit enhanced mechanical performance and offer interesting possibilities for structural applications.[29] In this work, the linear attenuation coefficients of an epoxy resin doped with nano-wo$_3$ and micro-wo$_3$ with the same portions have been calculated using the MCNP computer code. The results are compared with the experimental results reported by Dong *et al.*[24]

In this work, a simulation was carried out using the MCNP computer code, considering 50 wt% WO_3/E44 epoxy composite for micro and nano particles of tungsten oxide with sizes of 1 μm and 50 nm, respectively, adapted to the experimental work.[24] The formula of the epoxy resin E44 is $C_{21}H_{24}O_4$. For the definition of particle sizes of the fillers, lattice card was applied. A view of the lattice system is depicted in Fig. 1 for nano and micro sizes of WO_3 particles in the epoxy matrix. The magnification of this figure is such that for 6 μm × 6 μm (Fig. 1(a)) and 20 μm × 20 μm (Fig. 1(b)). The simulation geometry of validation calculations is exhibited in Fig. 2. WO_3 particles are located in the center of cubes in the epoxy resin lattice. A narrow straightforward beam of a gamma-ray source was defined in the front of the sample and perpendicular to it. To calculate the particle flux, one NaI scintillation detector has been used behind the sample of radius 3 cm and height of 0.02 cm and using F4 tally in one energy bin equal to defined energy of the source as the same as in the experiment.[24] According to the Lambert–Beer law, the linear attenuation coefficient of a material for gamma and x-ray are described as[30]

$$I = I_0 e^{(-\mu x)}, \tag{1}$$

where I is the intensity of photons transmitted across some distance x, I_0 is the initial intensity of photons, μ is the linear attenuation coefficient, and x is the distance traveled. Thus the linear attenuation coefficients can be calculated with

$$\mu = \frac{Ln(I_0/I)}{d}. \tag{2}$$

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The linear attenuation coefficients of WO_3/E44 epoxy samples were calculated for gamma rays at different energies, which have been obtained to be from 122.8 keV to 1330 keV.

The elemental weight fractions of the 50 wt% WO_3/E44 epoxy composite and physical characteristics of applied materials are presented in Tables 1 and 2, respectively.

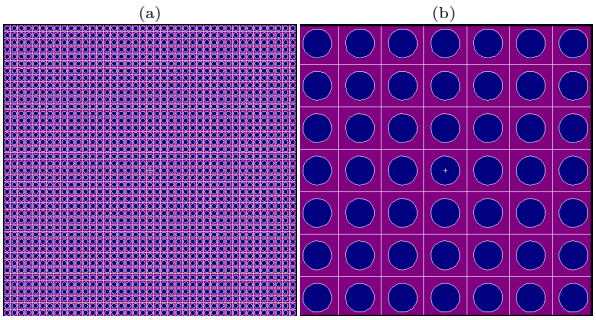

Fig. 1. Schematic view of the network of 50 wt% WO_3/E44 epoxy composite, in which WO_3 particles disperse uniformly in the epoxy matrix as spheres with radii of 50 nm (a) and 1 μm (b).

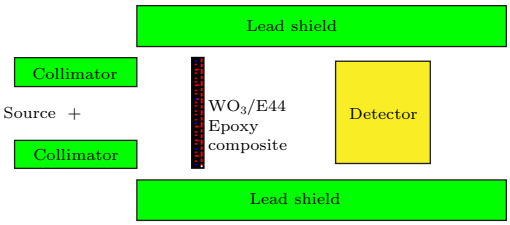

Fig. 2. Simulation geometry of validation calculations.

Table 1. Elements in the 50 wt% WO_3/E44 epoxy composite.

Element	Symbol	Atomic number	Atomic weight	Weight fraction
Hydrogen	H	1	1.00794	0.03553
Carbon	C	6	12.011	0.37047
Oxygen	O	8	15.9994	0.19751
Tungsten	W	74	183.84	0.39649

Table 2. Physical characteristics of applied materials at room temperature.[31]

Material	Density (g/cm^3)
WO_3	7.16
E44 epoxy	1.18
50 wt% micro-WO_3/E44 epoxy	2.18
50 wt% nano-WO_3/E44 epoxy	2.29

Figure 3 demonstrates the mass attenuation coefficient for 50 wt% WO_3/E44 epoxy composite at different energies from 1 keV to 5 MeV using XCOM.[32] Effective atomic number Z for 50 wt% WO_3/E44 epoxy composite calculated as 54.07 via XCOM.[32] Since the most effective shielding materials are those with high atomic numbers, and if the energy of the primary gamma rays is high, pair production within high-Z surrounding materials can give a significant yield of annihilation radiation,[33] this composite can be a suitable candidate for photon attenuation purposes. As can be easily seen from Fig. 3, there is K-shell in the energy of 70 keV, which belongs to tungsten. Figure 4 exhibits the relative increasing rate of linear attenuation coefficient (nano to micro) for 50 wt% WO_3/E44 epoxy composite at different energies. In this simulation, as can be seen from this figure, composites with nano-size particles of WO_3 show a larger number of linear attenuation coefficients in comparison with micro-size particles, which have been observed in the experiment.[24] To justify this phenomenon, it can be mentioned that nano size particles have cross sections greater than micro size particles. Thus collision probability of photons with tungsten particles in the nano size increases, which results in higher attenuation coefficients. The maximum discrepancy in the simulation results from the experimental ones is less than 5% for energies less than 778.6 keV, but in higher energies near 1330 keV, although the increase of linear attenuation coefficient is obvious, whereas the discrepancy is increased with the experimental work,[24] maybe as the work of Botelho *et al.*,[34] the nanostructured materials can be effectively used for low energy applications particularly radiological protection purposes.

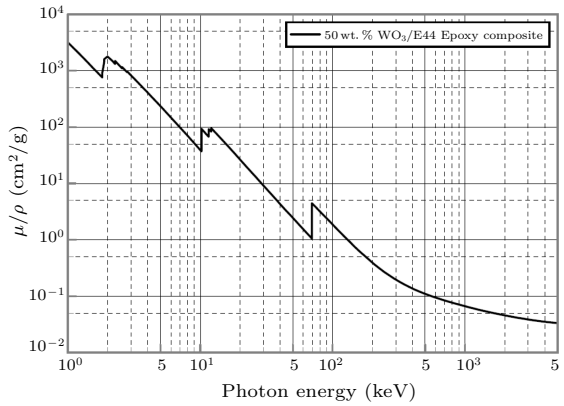

Fig. 3. Mass attenuation coefficient for 50 wt% WO_3/E44 epoxy composite at different energies using XCOM.

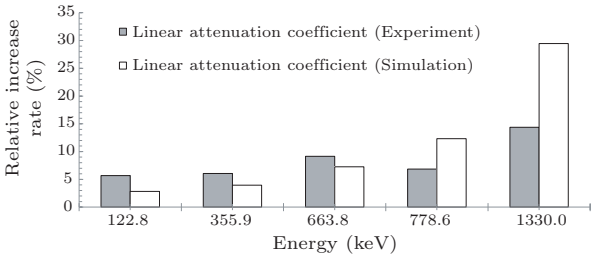

Fig. 4. The relative increasing rate of linear attenuation coefficient (nano to micro) and comparison with the experimental data.[24]

Figures 5 and 6 exhibit simulation results of the linear attenuation coefficient of 50 wt% WO_3/E44 epoxy composite at different energies for micro and nano structures, respectively, which are compared with the experimental data.[24] As can be seen from these figures, there is an acceptable correlation and agreement between the simulation and the experi-

ment.

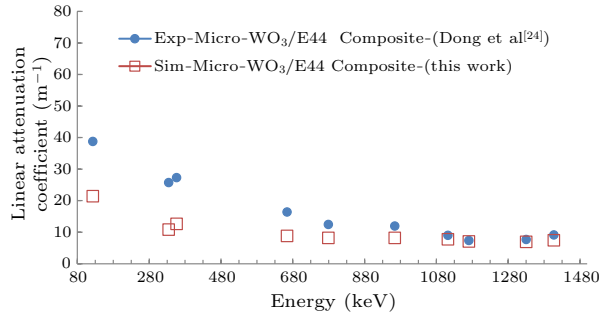

Fig. 5. Comparison of linear attenuation coefficient for micro 50 wt% WO_3/E44 epoxy composite at different energies for experiment[24] and our simulation.

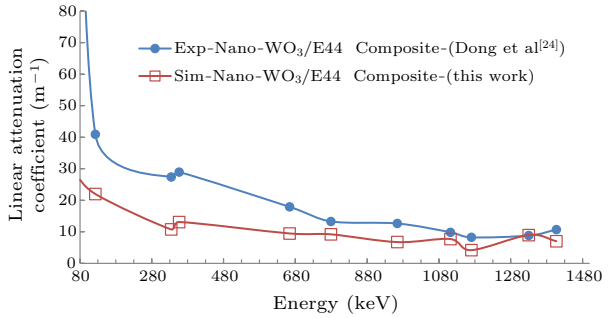

Fig. 6. Comparison of linear attenuation coefficient for nano 50 wt% WO_3/E44 epoxy composite at different energies for experiment[24] and our simulation.

In summary, the linear attenuation coefficient by nanostructured and microstructured of 50 wt% WO_3/E44 epoxy composites has been compared. The radiation shielding characteristics of this composite in micro and nano sizes of WO_3 particles are investigated in various gamma energies from 50 keV to 1.33 MeV via the MCNP code and are validated with the experimental data. The results show that nano size particles of WO_3 with 50 nm diameter exhibit a larger increase in linear attenuation coefficient in comparison with micro size particles with 1 μm diameter, which shows a good agreement with the experimental work.

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