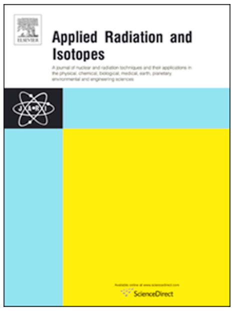

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# Random model for radiation shielding calculation of particle reinforced metal matrix composites and its application

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**Abstract:** The work aimed to calculate the radiation biological shielding performance of particle reinforced metal matrix composite (PRMMCs) using more reasonable model instead of conventional Uniform Filling Model, also attempted to provide a basis for the radiation shielding optimal design of such materials. Firstly, RSA (Random Sequential Adsorption) Model and GRM (Grid Random Model) were established based on MATLAB and Monte Carlo Particle transport program MCNP, and then advantages and disadvantages of them were compared. Later, the influences of metal matrix type, particle ($B_4C$) content, particle shape and particle shape parameters on the biological shielding performance of materials were calculated under different energy neutrons and different thickness shield using random models. Finally, the optimal aspect ratio of regular hexahedral $B_4C$ was calculated by Genetic Algorithm combined with MATLAB and MCNP. It indicated that GRM could be applied to radiation shielding calculation of PRMMCs.

**Keywords:** radiation shielding, MCNP Code, random model, PRMMCs, optimal design

## 1 Introduction

Not only good radiation shielding performance but also high thermodynamic and mechanical properties of shielding materials are necessary to meet requirements of the increasingly stringent nuclear service environment [1-3].Particle reinforced metal matrix composites (PRMMCs) have the very large potential to be used as both structural and functional shielding materials for its specific stiffness, strength and multiple reinforced particles[4,5].Due to its advantages of high thermal neutron capture cross section, high strength, low density and inactive chemical properties, $B_4C$ particle is widely used in shielding of nuclear industrial facilities [6-8]. Therefore, the present work focused on the $B_4C$ reinforced metal composites and investigated its shielding performance.

However, the difference in density will inevitably lead to gravity segregation problems in $B_4C$ reinforced metal matrix composites (such as iron, steel or copper). Meanwhile, the weldability of materials will also deteriorate with the increase of volume fraction of reinforced phase. For this, our research team proposed the concept of hollow body wrapped functional particle reinforced materials, which introduces matrix materials hollow body wrapped functional particle into the matrix and reserves the welding edge of the matrix, to try to overcome the problems. This means that the size of the hollow body will reach millimeter when considering the preparation process.

At present, the Monte Carlo Method is the conventional means to study the radiation shielding calculation and the Uniform Filling Model, which material components and elements are uniformly filled in the shield, is extensively adopted in the simulation calculation of the radiation shielding of materials [9-11]. To be fair, it is credible when the particle size of reinforced particles is much smaller, such as powder reinforced particles in polymer matrix shielding materials. However, for large reinforced particles, the calculation with this model will be not accurate even have a large error obviously. Therefore, a radiation shielding calculation model of PRMMCs is significant but scarce now. As far as investigation is concerned, W.R.Burrus' Model is the most representative model in spite of the drawback that it overlooked the absorption of neutrons by the matrix [12]. Some researchers successfully established a non-uniform model combining MCNP with MCAM[13] programs, named $B_4C$ particle size model, and applied to studying thermal neutron transmission coefficient and the mechanism of $B_4C$ particle size affecting the thermal neutron absorption performance, which was limited to thermal neutron calculation [14, 15]. In addition, some researchers received regular models, that particle arranged as simple cubic structure, body center cubic structure and face center cubic structure, to evaluate the shielding performance of metal foams materials [16].These models own their advantages but are not suitable of our calculation.

For the foregoing reason, to calculate the radiation shielding performance of PRMMCs accurately, the present work set up two kinds of suitable random model based on MATLAB and Monte Carlo Particle transport program-MCNP[17], Random Sequential Adsorption(RSA) Model and Grid Random Model (GRM). Thereinto, RSA Model was achieved based on random sequential adsorption (RSA) method that is a simple and effective means to generate random particle position and widely used in materials mechanical simulation by finite element method, but the spherical particle volume fraction is limited to a value lower than 38% for its theory flaw. GRM solved this problem and increased the value to 52.3% for sphere particle by meshing and choosing grid randomly. At the same time, GRM realized the calculation of irregular shape particle with bigger volume fraction. Learning from the simulation of materials mechanical property, metal matrix type, particle ($B_4C$) content, particle shape and particle shape parameters were considered to calculate the effect on materials' radiation biological shielding performance under given situations including of wide range of neutron energy from thermal neutron to 14.1MeV fast neutron and shielding thickness matched with the energy. Finally, GRM was applied to calculating the optimal aspect ratio of regular hexahedral $B_4C$ by genetic algorithm combined with MATLAB and MCNP program.

# 2 Methods of modeling and models

At present, the Uniform Filling Model based on Monte Carlo is still the mainstream to calculate radiation shielding performance of materials, which may be not accurate when the functional particle is large and may lead to shielding materials designed unpractical. In order to satisfy the radiation shielding analyses for larger particle reinforced metal matrix materials, this research realized two kinds of random model. Fig.1 intuitively shows the distinction between conventional Uniform Filling Model and present random model.

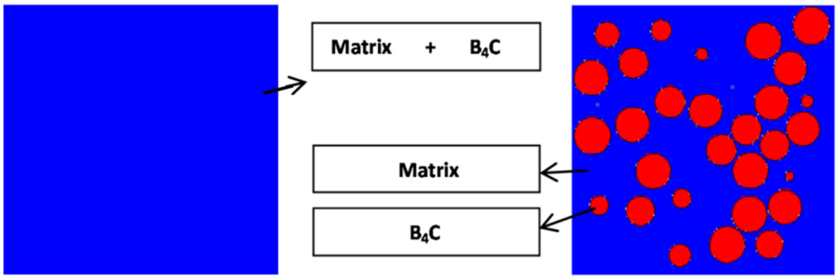

Fig. 1 Comparison betweenUniform Filling Model and random model

## 2.1 RSA Model

RSA Model was achieved based on RSA method by combining MATLAB(R2016a) with MCNP program, in which RSA means was used to generate the position parameters of particle distributed randomly in matrix and then parameters were employed to write the input file for MCNP program to run. The specific implementation way is that the first geometric center point was randomly generated in the considered volume, and then the next point was created in the remaining volume, and the points were produced circularly until the volume fraction occupied by particles reached the set value. The new point should satisfy following formulas,

$$|x_{min} - R_{max}| \leq x_i \leq |x_{max} - R_{max}|$$
$$|y_{min} - R_{max}| \leq y_i \leq |y_{max} - R_{max}|$$
$$|z_{min} - R_{max}| \leq z_i \leq |z_{max} - R_{max}|$$
$$d \geq R_{max}$$
$$sphere: R_{max} = 2 \times r; cylinder: R_{max} = 2\sqrt{r^2 + \left(\frac{h}{2}\right)^2}; cube: R_{max} = \sqrt{3}a (1)$$

Where$x_{min}$,$y_{min}$,$z_{min}$,$x_{max}$,$y_{max}$and$z_{max}$are the geometry boundary, $d$is the distance between new point and former points, $R_{max}$is the maximum central distance that the particles do not overlap with each other, $r$is the radius of sphere and the bottom radius of cylinder, $h$is the height of cylinder, $a$is length of side of cube. Fig.2 presents the final RSA Model plotted by Vised Program matched with MCNP program, which can only draw two-dimensional cross-section picture. The single particle size of sphere and cylinder are showed obviously in Fig. 2(a) and Fig. 2(b). What is worth mentioning is that this model can also be successfully applied to calculating the radiation shielding of hollow ball foam materials and cavitation type foam materials showed in Fig. 2(c) and Fig. 2(d).

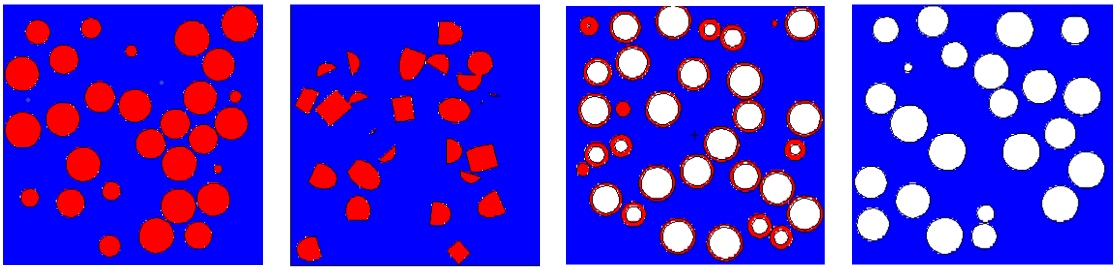
(a) (b) (c) (d)

Fig. 2RSA Model plotted by Vised Program: (a) Single size spherical particle
(b) Cylindrical particle (c) Hollow ball foam materials (d) Cavitation type foam materials

## 2.2 Grid Random Model

Similarly, the establishment of GRM was also divided into two steps: generating parameters of particle and writing input file. Firstly, the mesh was divided into proper size that is related to the size of reinforced particles. Then a random grid was selected and the central point of the grid was used as the geometry center of the reinforced particle. The non-overlapping grids were repeatedly selected successively until the particle volume fraction reached the set value. Fig. 3 is the cross-section picture of GRM drawn by the Vised Program. It must be mentioned that central axis orientation of cylinder and cube particles is parallel to the one of coordinate axis.

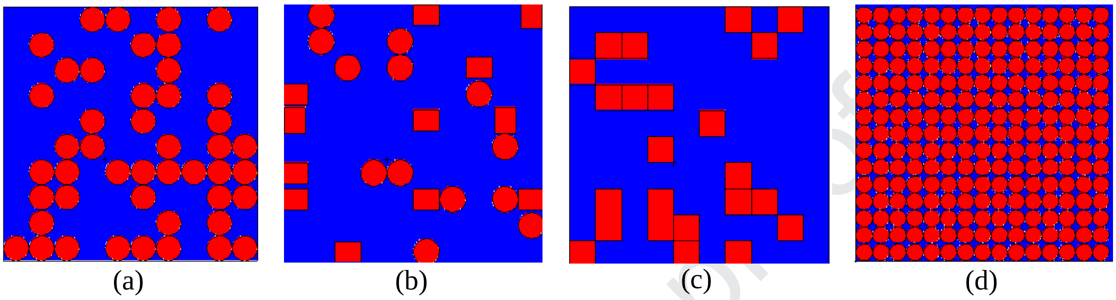
(a) (b) (c) (d)

Fig. 3GRM plotted by Vised Program: (a) Spherical particle (b) Cylindrical particle (c) Cubic particle (d) The entire grid is occupied by particle

## 2.3 Comparison between two random models

Considering that two models will be used in the optimization calculation of PRMMCs, the single modeling time of the two random models was respectively analyzed (sphere: SPH;Cylinder: RCC), as shown in Fig.4.

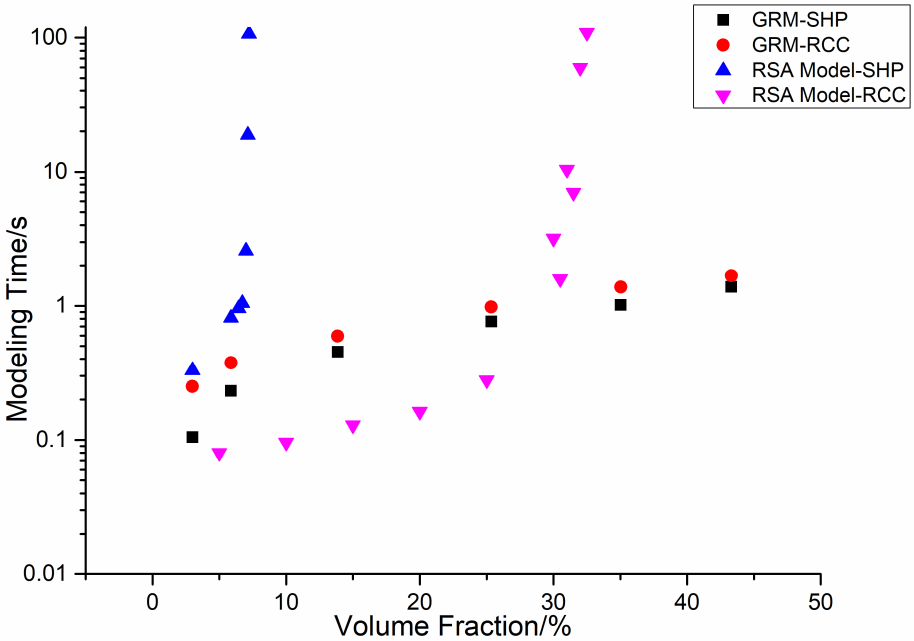

Fig. 4 The relationship between modeling time and particle volume fraction

In general, the modeling time of GRM is much less than RSA Model. It can be seen in detail that the modeling time of RSA Model increases rapidly with the increase of particle volume fraction, especially for cylinder particle. However, the modeling time of GRM also increases with the increase of particle volume fraction, but the increase is slight and even if the volume fraction reaches 45%, the modeling time do not exceed 2 seconds. What is more important is that the modeling time of cylinder particle for GRM is also very small, it means that GRM is also suitable to non-spherical particle.

The main reason of the difference between these two models is that RSA Model used conservative values $R_{max}$ to determine all non-overlapping particles when generating particle parameters, so the space utilization rate of considered volume is low .Therefore, with the increase of particle volume fraction, the modeling time will increase exponentially. Because the $R_{max}$ of cylinder is larger and the space utilization is much lower, the achievable volume fraction is smaller than the sphere. However, GRM sacrificed a certain degree of randomness by dividing grids, making the modeling time much smaller than RSA Model. Meanwhile, by specifying the orientation directions of cylinder and cube, the space utilization rate was improved, so modeling of larger volume fraction of particles can be achieved.

On the whole, for a small volume fraction (< 30vol. %) of single size spherical particles reinforced composite material, RSA Model is more reasonable and accurate for its much randomness. However, for larger volume fraction of single size spherical particles and non-spherical particles reinforced composite materials, GRM is more efficient, especially for optimization design.

## 2.4 Comparing Grid Random Model with previous model

Some researchers have established a $B_4C$ particle size Model which is similar to random model in this paper, so GRM was adopted to carry out the same calculation based on the relevant parameters in Fig.2 of the literature[14], the size of the shield is 1mm × 0.1mm × 1mm, the diameter of $B_4C$ ranges from 63 μ m to 90 μ m. Then the results were compared, as shown in Fig.5. Because of the random position of particle, GRM owns the inherent model errors, each data point was calculated 10 times and averaged.

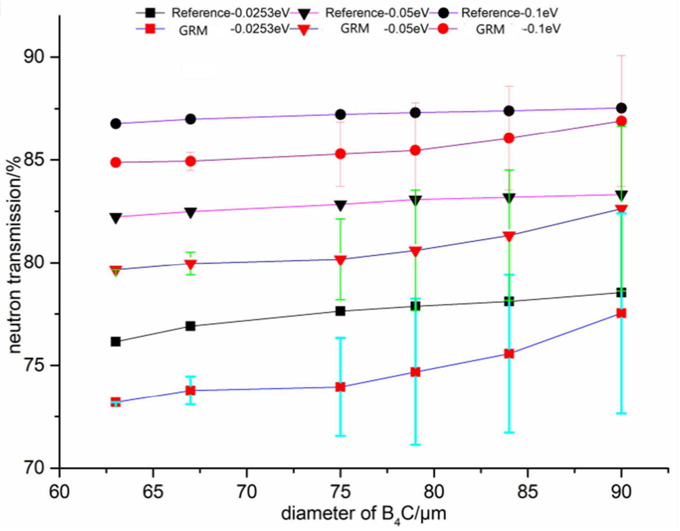

Fig.5 Comparison between GRM and $B_4C$ Particle Size Model in the reference

Fig.5 displays that the calculated results using GRM are slightly smaller, about2%-5%, than those in the literature. There are two main reasons. First, the specific size of the surface source and body detector was estimated for they are not clearly described in the literature. Secondly, the shield is thin enough to fill only one layer of $B_4C$ particle in the literature, which would lead to great randomness error. If model errors of the GRM were taken into account, the results in the literature were within the range of uncertainty. It was noted that the 63μm designed in the literature is just $B_4C$ completely covered with shield, as shown in Fig. 3(d). Obviously, there were only statistical errors and no model errors for GRM, so, the uncertainty was very small.

# 3 Simulation calculation

## 3.1 The whole calculation model

Based on random models, the influences of metal matrix type, particle ($B_4C$) content, particle shape and particle shape parameters on the biological shielding performance of materials were calculated under different energy neutrons. And size of the shield was matched with the different neutron energy. The whole calculation model is shown in Fig.6.

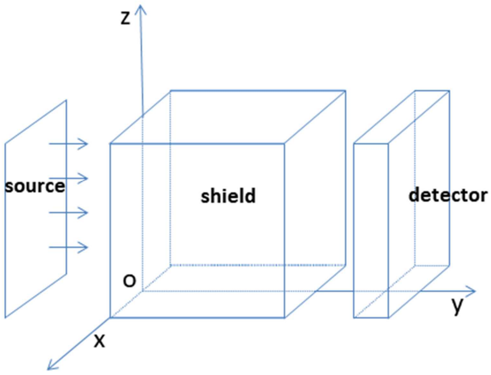

Fig.6 The whole calculation model

Among them, the shield was the random model described above. Because the random distribution of particles would lead to a certain model error in each calculation result, the radiation source was chosen a surface source of the same size as the front surface of the shield, and the front surface of the body detector was the same size as the rear surface of the shield. In this work, the biological shielding performance of the shield was considered, so, the total dose equivalent behind the shield was calculated, including the neutron dose equivalent and the secondary gamma dose equivalent. And the lower the dose equivalent is, the better shielding performance of the shield.

## 3.2 Results and discussions

### 1) Matrix type and particle contents

It is known to all that aluminum, iron and copper are commonly used metal matrix materials, and alloy materials are better than pure metal materials in mechanical and thermal properties. Therefore, the shielding properties of $B_4C$ reinforced alloy matrix composite materials are compared based on GRM, the matrix is followings: Al356.2, 316stainless steel and casting brass ZCuZn26Al4Fe3Mn3.Among them, $B_4C$ was spherical and shield thickness was selected as the length of about 5 mean free paths of each energy neutron in materials.

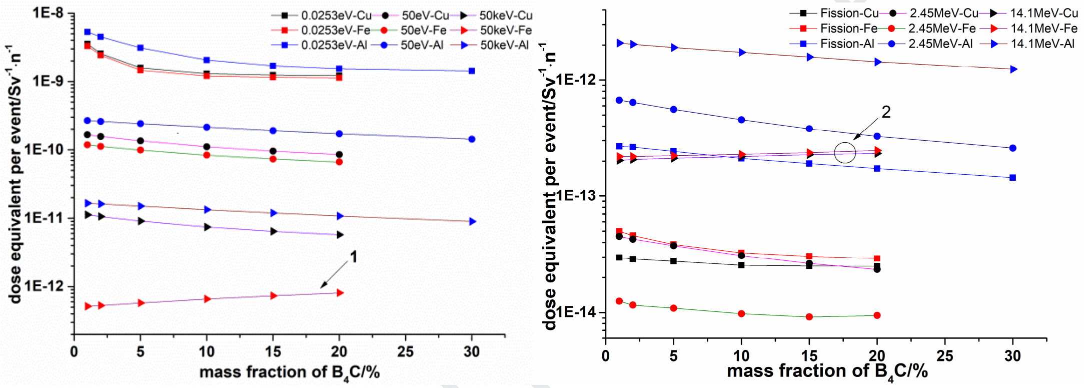

Fig.7 Comparison between various matrix composite materials

It can be conclued that except for 50keV (curve 1) and 14.1MeV (curve 2), the neutron shielding performance of each material in each energy increases with the increase of $B_4C$ mass fraction. In the case of thermal neutrons and low-energy neutrons, it is mainly the absorption of thermal neutrons by $^{10}B$, which improves the shielding performance of materials.In the case of intermediate neutrons, fission neutrons and fast neutrons, the proportion of thermal neutrons moderated by the matrix material gradually decreases, so $^{10}B$ plays a limited role, but the moderating of B and C elements still improves the shielding performance to a small extent. However, when the nuetron energy is too high, the moderating effect of B and C will be smaller than that of the matrix materials, so the shielding property of the material weaked with the increase of $B_4C$, as shown in the curve 2. The curve 1 shows that the shielding property of stainless steel decreases with the increase of $B_4C$, because the neutron of 50keV is in the resonance energy region of iron, and this region should be the trough region of the microscopic cross section.And the result is opposite when the nuetron energy is changed 50keV to 70keV, which was also checked.

In general, the shielding performance of aluminum alloy matrix comopsite is much lower than that of stainless steel and casting brass matrix composites.The shielding performance of stainless steel matrix composites is better than that of casting brass matrix composites when the source is thermal neutron, low energy, intermediate energy and 2.45MeV neutron, and that is opposite for fission and 14.1MeV neutron. The result is consistent with the rule of neutron microscopic cross section in matrix materials, shown in table 1.

**Table 1**The neutron microscopic cross section of main metal element (from ENDF database[18])

| Energy | Element | | |
|---|---|---|---|
| | Cu | Fe | Al |
| 0.0253eV | 11.77 | 15.99 | 1.69 |
| 50eV | 7.48 | 11.41 | 1.42 |
| 50keV | 2.36 | 3.88 | 2.29 |
| fission | 3.05 | 2.73 | 2.22 |
| 2.45MeV | 3.11 | 3.31 | 2.09 |
| 14.1MeV | 2.94 | 2.56 | 1.74 |

## 2) Particle shape

Based on GRM, the different shapes $B_4C$ under the same volume were calculated (sphere: SPH;Cylinder: RCC; cube: RPP) on shielding properties of different alloy matrix composites in different neutron energy, shown in Fig.8. The thickness of the shield was selected as about 5 mean free path lengths. It must be mentioned that the bottom diameter of the cylinder was same as the diameter of the sphere, and the central axis of cylinder and cube was randomly selected to be parallel to one of the three coordinate axes (x/y/z).

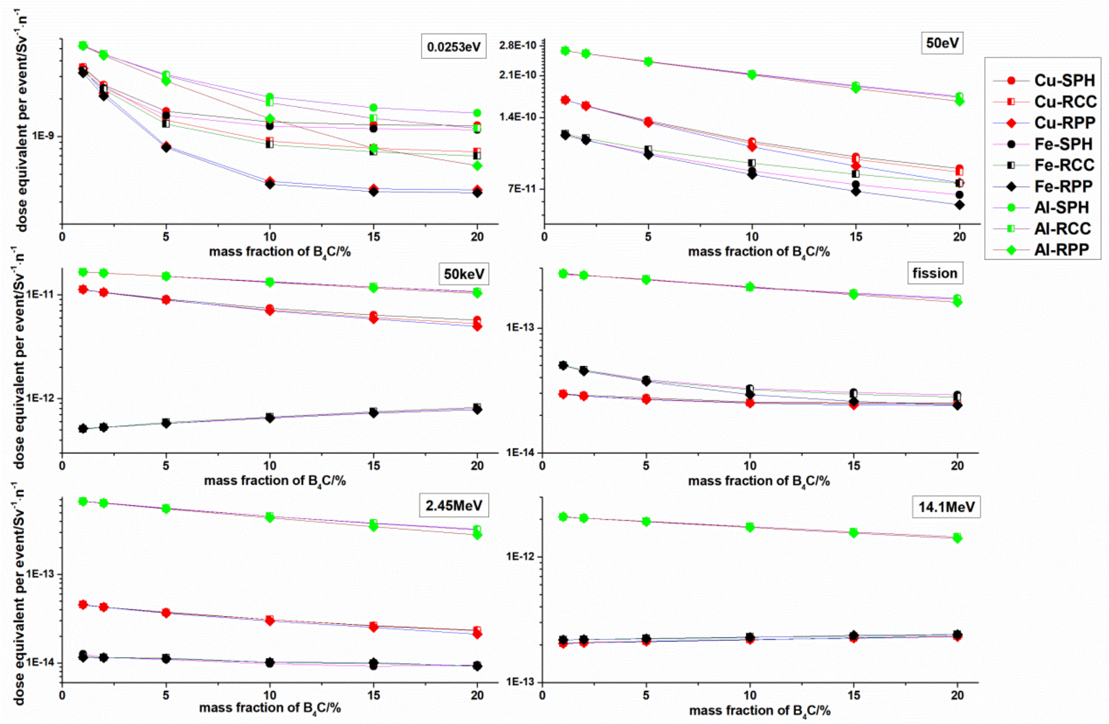

Fig.8 The influence of different shapes $B_4C$ on the shielding performance

As you can see that the materials reinforced by cubic $B_4C$ has the best shielding performance while the materials reinforced by spherical $B_4C$ is the worst, which is same with the result in other works[11]. This can be explained as follows: assuming that the thermal neutron is completely absorbed by $B_4C$ upon contact with the surface of $B_4C$ particle, then the effective cross section of the thermal neutron interacting with $B_4C$ is proportional to the total surface area of $B_4C$ in the shield. For sphere, cylinder and cube under the same volume, the total surface area is as following formulas,

$$S_{TSPH}=4\pi r^2\frac{wV}{V_0}$$
$$S_{TRCC}=4\frac{2}{3}\pi r^2\frac{wV}{V_0} \quad (2)$$
$$S_{TRPP}=6\left(\frac{4}{3}\pi\right)^{2/3}r^2\frac{wV}{V_0}$$

Where $V$, $w$,$V_0$are the volume of the shield, the volume fraction of $B_4C$ and the volume of $B_4C$. Clearly, $S_{TRPP}>S_{TRCC}>S_{TSPH}$ ,which is consistent with the rule of calculation. And the differences are obvious when the source is thermal neutron, about 70%. For other energy neutrons, the differences are no more than 10% and it is less than 3% for 14.1 MeV neutron.

At the same time, it is clear that the shielding performance of the materials is affected by both particle shape and matrix materials, and it is more obvious when the neutron is 0.0253eV. From the crossing line of the 0.0253eV neutron, it can be seen that the shielding performance of cube $B_4C$ reinforced Al matrix materials is better than sphere and cylinder $B_4C$ reinforced Cu and Fe matrix materials while the same shape $B_4C$ reinforced Cu and Fe matrix materials is far better than Al matrix materials.

## 3) Particle shape parameter

Based on the random models, the influence of particle shape parameters on the shielding performance of the casting brass ZCuZn26Al4Fe3Mn3 matrix materials was simulated and calculated, that the particle size was considered for spherical $B_4C$ and aspect ratio was taken into account for cylinder and regular hexahedron $B_4C$.

As mentioned above,RSA Model can be used for calculation of composite materials reinforced by spherical particle with small volume fraction while GRM is more suitable for composite materials reinforced by special-shaped particles. Therefore, RSA Model was used for calculation of spherical $B_4C$ with the 10wt.% while the GRM was adopted to cylindrical and regular hexahedral $B_4C$ with the 20 wt.%, at the same time, the volume of particles was same.

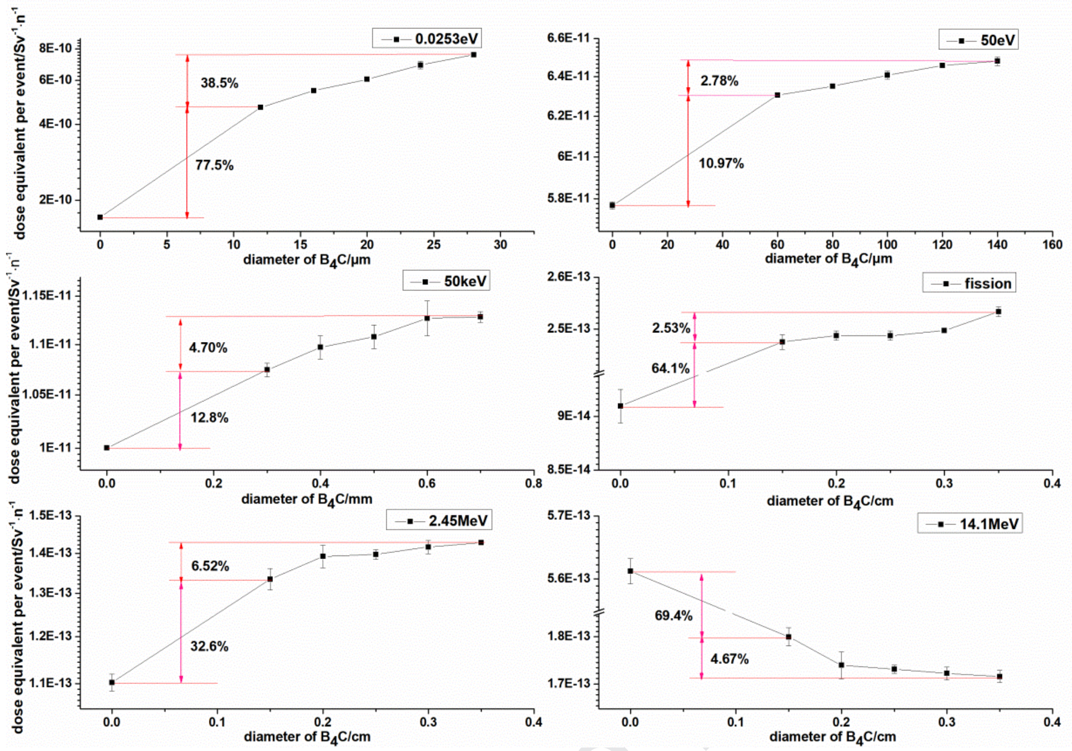

Fig.9 Effect of particle size of spherical $B_4C$ on shielding performance of materials (The boron carbide diameter size is 0 represents the data of Uniform Filling Model)

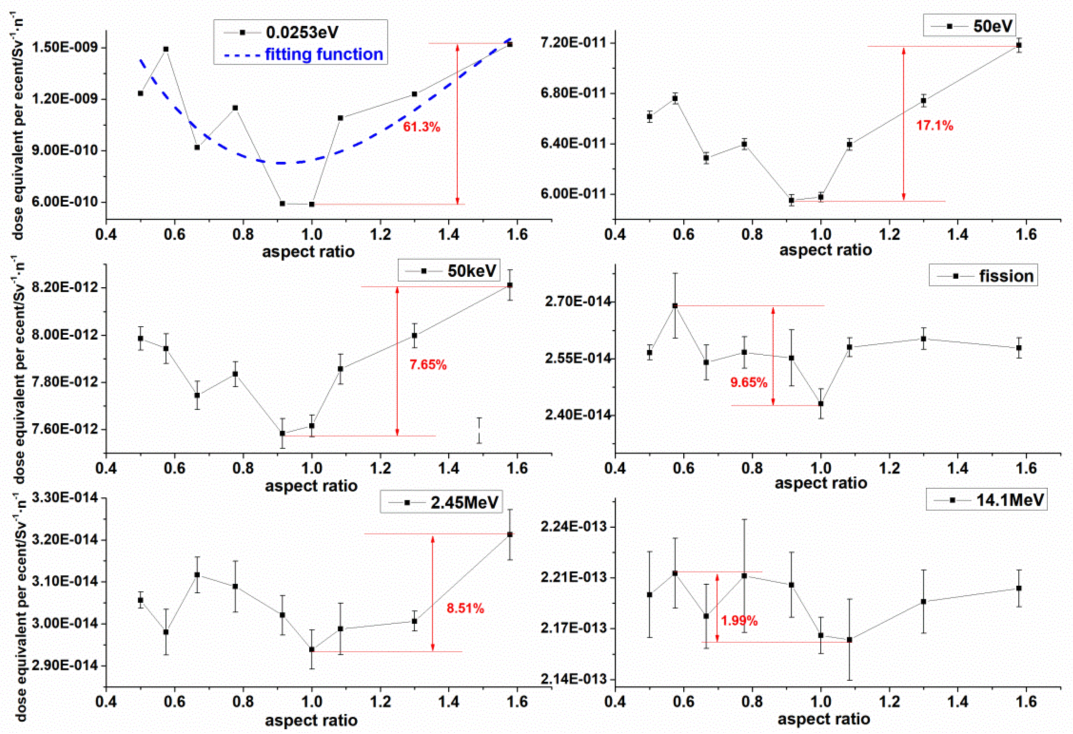

Fig.10 Effect of aspect ratio of cylindrical $B_4C$ on shielding performance of materials

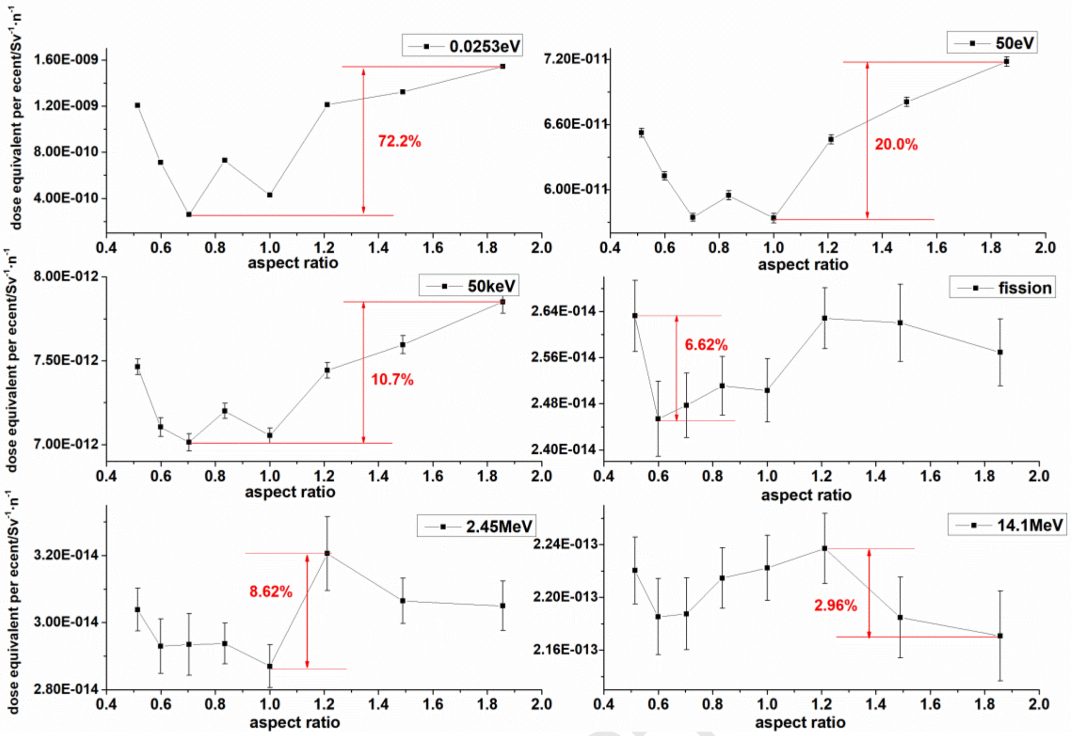

Fig.11 Effect of aspect ratio of regular hexahedral $B_4C$ on shielding performance of materials

As can be seen from the Fig.9, Fig.10 and Fig.11, the neutron shielding performance of the shield improves with the decrease of $B_4C$ particle size for spherical $B_4C$, which can also be explained by the effective cross section, as formula (3) shows.

It can be seen that the total effective cross section is inversely proportional to the radius of spherical $B_4C$, what means that the neutron shielding performance of the material is inversely proportional to the radius of spherical $B_4C$. However, when neutron energy is 14.1MeV, the neutron shielding performance of the materials depends on metal matrix by inelastic collision more than $B_4C$ by absorption capture, which means the larger the total effective cross section of $B_4C$ is, the worse the materials shielding performance is. So, the neutron shielding performance of the material reduces with the decrease of $B_4C$ particle size for spherical $B_4C$ when neutron energy is 14.1MeV. In addition, Fig.9 shows a fact that the results of GRM are larger than those of Uniform Filling Model, which verifies that Uniform Filling Model is not suitable for PRMMCs.

$$\frac{S_{1tol}}{S_{2tol}}=\frac{S_1\cdot n_1}{S_2\cdot n_2}=\frac{4\pi r_1^2 V/\left(\frac{4}{3}\pi r_1^3\right)}{4\pi r_2^2 V/\left(\frac{4}{3}\pi r_2^3\right)}=\frac{r_2}{r_1} \tag{3}$$

Generally, with the increase of the aspect ratio of cylinder and regular hexahedral $B_4C$, the shielding performance of the materials shows a trend of increasing first and then decreasing. The blue fitting function curve in Fig.10 is a quadratic polynomial fitting and it can show the tendency obviously. It can be seen that it is better when the aspect ratio reaches approximately 1.0. As we can see that there is a step fluctuation when it decreases and increases. It means there are also other factors to influence the shielding performance besides the aspect ratio. For the limit of GRM, the central axis of cylinder and regular hexahedral $B_4C$ is not in random direction and it was just randomly parallel to one of the three coordinate axes (x/y/z), which was different from spherical $B_4C$, it may influence the dislocation occlusion between $B_4C$ particles and influence the scattering of neutron. Therefore, there is a step fluctuation.

## 4) Optimal design of aspect ratio

It is no linear relationship between shielding performance and aspect ratio for cylindrical and hexahedral $B_4C$ reinforced materials, as shown in Fig.10 and Fig.11. Therefore, in a certain aspect ratio range (0.5-1.58), the aspect ratio of hexahedron $B_4C$ was optimized based on genetic algorithm by using MATLAB combined with MCNP programs. Where, the source was thermal neutron, the matrix was casting brass ZCuZn26Al4Fe3Mn3, the shield thickness was 3 mean free paths and the mass fraction of $B_4C$ was 10% because of considering the optimization time. The total dose equivalent behind the shield, about $10^{-9}$ order of magnitude, was the objective function.

In the optimization calculation process, the calculation will stop when the difference between the objective function values of each generation is less than $10^{-6}$, which will result in insufficient optimization. Therefore, objective function value was multiplied by $10^{9}$ to be the Fitness value which was shown as ordinate in Fig.12.

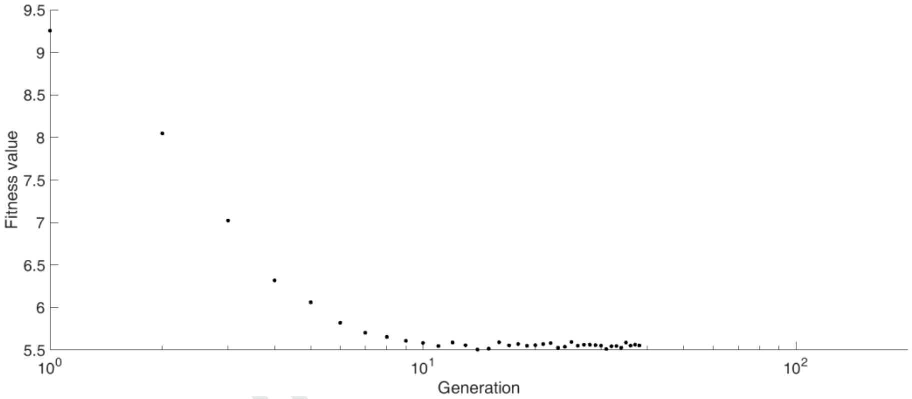

Fig.12 Schematic diagram of optimization process

The Fig.12 displays the schematic diagram of optimization process, it can be seen that the fitness value gradually diminishes until the minimum value in about 40 generations. Finally, the optimizing aspect ratio is 0.902. In addition to this, it can also verify that GRM can be applied to optimizing.

# 4 Conclusions

In this paper, two kinds of suitable and accurate model, RSA Model and Grid Random Model (GRM), for radiation shielding calculation of PRMMCs were established. The effect of matrix type, particle ($B_4C$) content, particle shape and particle shape parameters on materials' radiation biological shielding performance under different energy neutrons were calculated and the optimal aspect ratio of regular hexahedral $B_4C$ was obtained. From the results, several main conclusions are provided:

(i)RSA Model is more reasonable and accurate for a small volume fraction (< 30vol. %) of spherical particles reinforced composite material. GRM is more efficient for larger volume fraction of spherical particles and non-spherical particles reinforced composite materials, especially for optimization design.

(ii)Except for 50keVand 14.1MeV neutrons, the shielding performance of every matrix materials increases with the increase of $B_4C$ mass fraction.The shielding performance of aluminum alloy matrix comopsite is much lower than that of stainless steel and casting brass matrix composites.The shielding performance of stainless steel matrix composites is better than that of casting brass matrix composites when the source is thermal neutron, low energy, intermediate energy and 2.45MeV neutron, and that is opposite for fission and 14.1MeV neutron.

(iii)The materials reinforced by cubic $B_4C$ have the better shielding performance than same volume cylindrical $B_4C$ reinforced materials while the materials reinforced by spherical $B_4C$ are the worst. This is consistent with their superficial area.

(iv)The neutron shielding performance of the shield improves with the decrease of particle size for spherical $B_4C$. For cylindrical and regular hexahedral $B_4C$, the shielding performance is better when the aspect ratio reaches approximately 1.0, and the optimizing aspect ratio is 0.902 for regular hexahedral $B_4C$ when the matrix is casting brass and the source is thermal neutron.

(v) For $B_4C$ reinforced metal matrix radiation shielding materials, as many as possible $B_4C$, the smaller particle size spherical $B_4C$ or cubic $B_4C$ can improve the shielding performance of the material.

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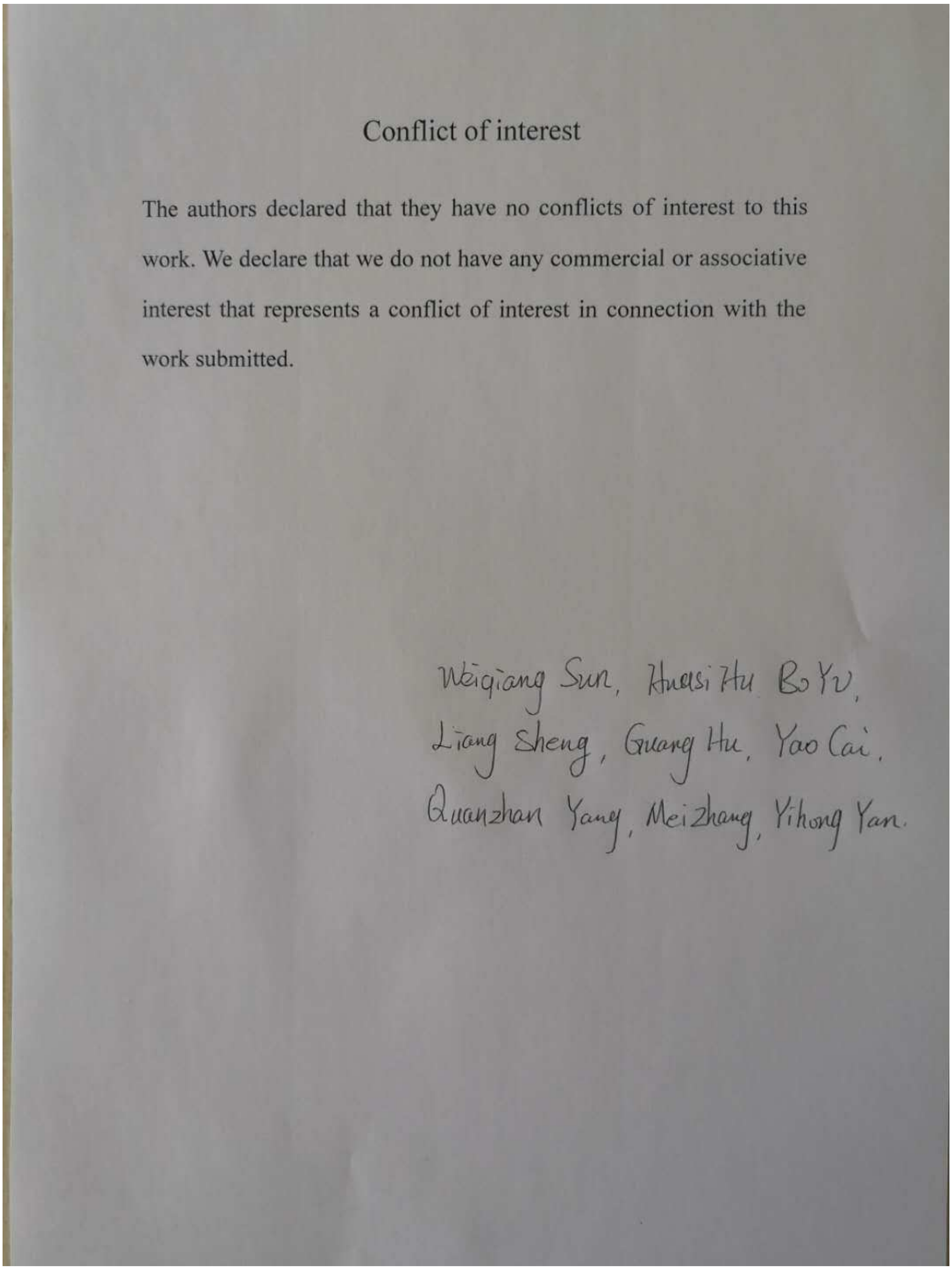
## Highlights:

i. Two kinds of suitable random model were established for radiation shielding calculation of particle reinforced metal matrix composites.
ii. Metal matrix type, particle content, particle shape and particle shape parameters were all considered to calculate the effect on materials’ radiation shielding performance.
iii. The optimal aspect ratio of regular hexahedral $B_4C$ was calculated by Genetic Algorithm combined with MATLAB and MCNP.



# Conflict of interest

The authors declared that they have no conflicts of interest to this work. We declare that we do not have any commercial or associative interest that represents a conflict of interest in connection with the work submitted.

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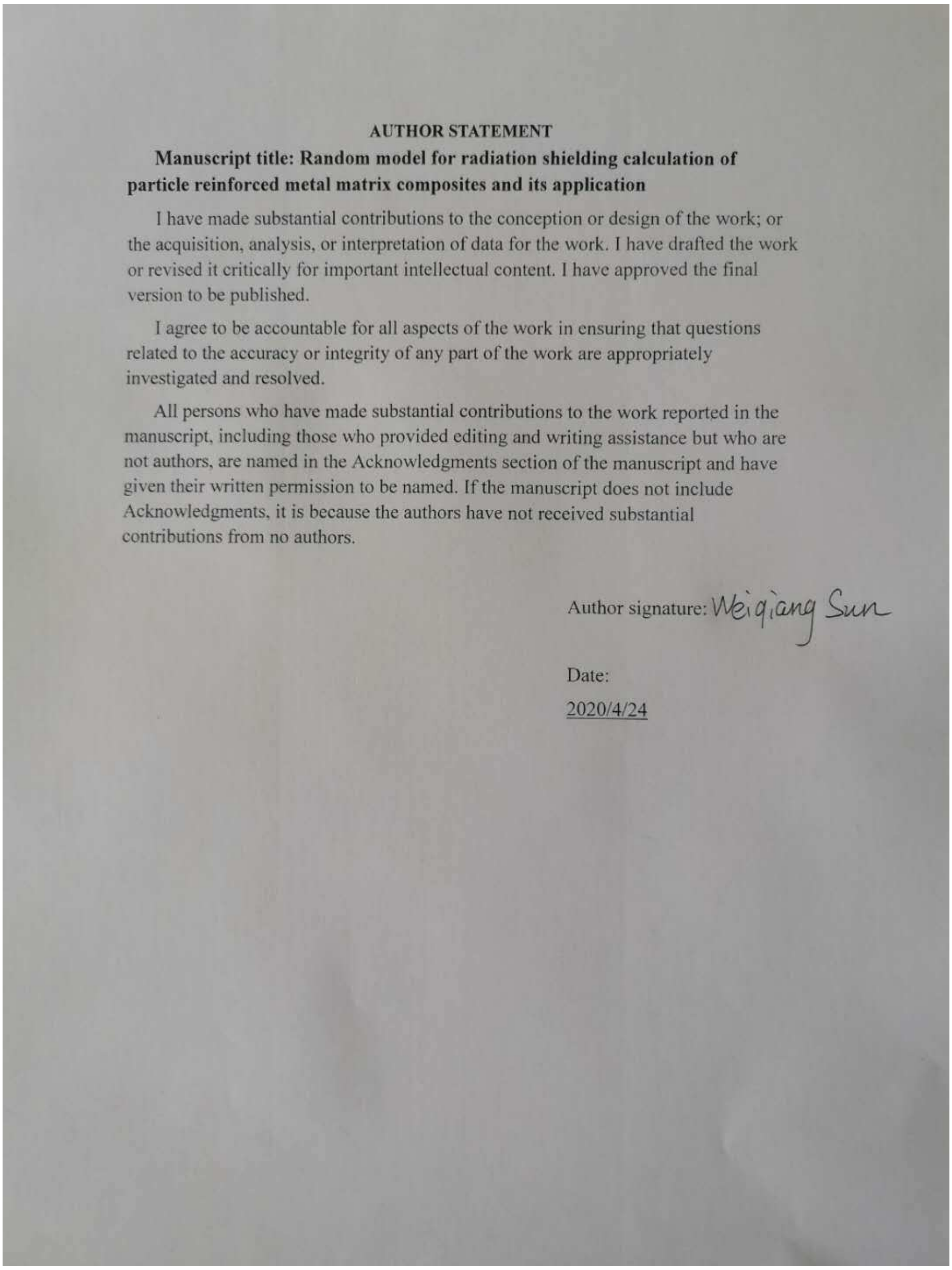

## AUTHOR STATEMENT

**Manuscript title: Random model for radiation shielding calculation of particle reinforced metal matrix composites and its application**

I have made substantial contributions to the conception or design of the work; or the acquisition, analysis, or interpretation of data for the work. I have drafted the work or revised it critically for important intellectual content. I have approved the final version to be published.

I agree to be accountable for all aspects of the work in ensuring that questions related to the accuracy or integrity of any part of the work are appropriately investigated and resolved.

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