Communication

Investigating the Effect of SiCp Particle Shape on the Mechanical Behaviors of SiCp/WE43 Magnesium Matrix Composites by Finite Element Simulation

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Abstract: Previous results reported that SiCp (Silicon Carbide particles) particle doping proved to be effective in enhancing the wear performance of WE43 magnesium alloy. In this work, finite element simulation was employed to investigate the effect of SiCp particle shape on the mechanical behaviors of SiCp/WE43 magnesium matrix composites. SiCp particles underwent larger load internally and a smaller plastic deformation under tensile loading, leading to the enhanced strength and stiffness of the composites. Polygonal SiCp particles provided a better enhancement in strength for the composites than round SiCp particles, but the enhancement in stiffness was opposite. Meanwhile, the damage is likely to initiate at the interface between the matrix and particle, at the location of the highest stress concentration. This phenomenon was more prominent in polygonal particle-reinforced composites. These current findings provide a comprehensive understanding of the effect of SiCp particle shape on the mechanical behaviors of magnesium matrix composites.

Keywords: SiCp doping; magnesium matrix composites; strength; stiffness; finite element simulation

1. Introduction

Particle-reinforced metal matrix composites (PRMMCs) are becoming a hot research topic, and they are beginning to replace single-component alloy materials due to their superior mechanical properties [1–3]. WE43 magnesium alloy has a wide range of prospective applications in marine engineering and vehicle engineering due to its good thermal conductivity and excellent damping properties. However, the poor wear resistance of magnesium alloy greatly affects its reliability and service life. Magnesium matrix composites reinforced by SiCp (Silicon Carbide particles) particles have high specific strength and high specific stiffness, which make them a promising material for development [4]. Hajo Dieringa [5] reported that the nanoparticle-reinforced magnesium composites were expected to enjoy strengthening due to the grain refinement described in the Hall–Petch relation. However, it is difficult to quantitatively analyze the effect of microscopic factors (e.g., particle shape, size, content) on the strengthening and damage behavior of the particle-reinforced composites by experimental studies and mesomechanics [6,7]. Up to now, the effect of meso-scale characterization on the mechanical properties of PRMMCs is mainly based on theoretical and numerical simulations [8–10]. Shao et al. [11] reported that the yield strength of TiC/AZ91 magnesium matrix composites decreased with the increase in TiC particle size for the single size particle-reinforced composites.

Our previous results confirmed that SiCp doping was effective in enhancing the bearing capacity of WE43 matrix alloy, but also that it greatly improved its wear resistance [12]. However, the effect of SiCp particles on the mechanical behaviors of SiCp/WE43 magnesium matrix composites is still largely unclear. In this work, two-dimensional plane strain
unit cell finite element models for composites doped with different SiCp particle shapes were established using the finite element method. The stress and strain distribution within the composites and tensile stress–strain curves were analyzed to investigate the mechanical behaviors of these composites. The purpose of the present work is to provide a direct description of the effect of SiCp particle shape on the mechanical properties of SiCp/WE43 magnesium matrix composites.

2. Materials and Methods

In this section, the representative volume element (RVE) was used to establish the relationship between the macroscopic properties and the microstructure of the composite.

2.1. Finite Element Model

In order to reduce the number of calculations and improve computational efficiency, the two-dimensional plane strain unit cell finite element models for SiCp/WE43 magnesium matrix composites were established using the finite element method as an alternative to the three-dimensional physical model. They are based on the assumption of the “regular distribution” of SiCp particles (SiCp particles do not overlap and touch each other within the composites [13–15]). Four SiCp particles were doped inside the model in this work because the deformation behavior of the multi-particle-reinforced composite is similar to that of the single-particle-reinforced composite and the deformation effect is more obvious. SiCp particles were modeled into a square of 50 μm × 50 μm. Define the model width direction as the X direction and the model thickness direction as the Y direction. S_11 was defined as the stress component in the X direction, S_{max} was defined as the maximum principal stress, and PEEQ was defined as the equivalent plastic strain. Figure 1 shows all particle shape and size information. SiCp particles were shaped into circles, equilateral triangles, squares, and regular pentagons [16]. The radius of round particles is 5 μm; therefore, the area fraction (the ratio of the total area of the particles to the total area of the model [17]) of inclusions is 12.56%. The sizes of the other three shapes of SiCp particles were calculated according to the principle of “the same area fraction as the circular particles”.

![Figure 1. Schematic diagram of the composite models with different shapes.](image)

2.2. Basic Assumptions and Material Parameters

In order to facilitate the analysis and calculation, the following assumptions are made for the finite element model of the SiCp/WE43 magnesium matrix composites:

1. The interface between the particle and matrix reaches a perfect interface state and no penetration occurs. In addition, no sliding is allowed [18].
The SiCp/WE43 magnesium matrix composites are isotropic elastic–plastic bodies in the two-dimensional plane state. The plastically yielded criterion is simplified in that composites first undergo plastic deformation in the region where the equivalent stress exceeds their yield strength, neglecting the microstructural defects of the composites [19].

In addition, the stress–strain curve of the composites satisfied bilinear isotropic hardening. The material parameters of the matrix alloy and the SiCp particle required in the finite element simulation include: density (\(\rho\)), elastic modulus (E), Poisson’s ratio (\(\mu\)), yield strength (\(\sigma_S\)), and tangent modulus (\(E_T\)). We obtained some of the parameters of the material through experiments and calculations in previous results and, combined with the data query, the final set of material parameters are shown in Table 1.

### Table 1. Mechanical parameters of the matrix alloy and SiCp particle [3,12,20].

| Material | E (GPa) | \(\sigma_S\) (GPa) | \(E_T\) (GPa) | \(\mu\) |
|----------|---------|---------------------|----------------|-------|
| WE43     | 44.2    | 0.188               | 1.56           | 0.27  |
| SiCp     | 410     | 0.35                | 0.192          | 0.14  |

#### 2.3. Element Types and Meshing

The particles and matrix were meshed with 4-node bilinear plane strain quadrilateral reduced integration elements. The mesh was a 2D quad-dominated free mesh, and mapped meshing was used where appropriate to improve mesh quality. While ensuring mesh convergence, the finer the mesh division, the smaller the effect on the finite element simulation results. The maximum element size was 0.462. The number of elements in the model was 11,825 and the number of nodes was 11,847.

#### 2.4. Loads and Boundary Conditions

For a finite element model with good geometric symmetry, the periodic boundary condition can impose the equal displacement boundary condition. That is, the equivalent displacement of the corresponding nodes of the two opposite surfaces is considered to be equal, which is reflected in the finite element calculation as coupling the displacements of the two symmetry faces. Therefore, in this paper, a simplified equal-displacement boundary condition, i.e., equivalent displacement on a fixed boundary, is used to make the periodic boundary condition forcibly satisfied. The displacement boundary conditions were used for uniaxial tensile simulation of composites in the X-direction [21–23]. \(U_1\) represents the displacement along the X direction. \(U_2\) represents the displacement along the Y direction. \(U_{R3}\) represents the rotation around the Z direction. Nodes on the left of the model were set to \(U_1 = U_{R3} = 0\). The lower left node of the model was set to \(U_1 = U_2 = U_{R3} = 0\). Nodes on the right of the model were displaced along the positive X direction. The maximum displacement was 5 \(\mu\)m, which was 10% of the length of the model [24]. The lower right node of the model was set to \(U_2 = 0\) and \(U_1 = 5\). Taking the round particle-reinforced composite as an example, the schematic diagram of the periodic boundary conditions is shown in Figure 2, and the expression for the periodic boundary condition is:

\[
\begin{align*}
  u_{BC}(y) - u_B &= u_{AD}(y) - u_A \\
  u_{DC}(x) - u_D &= u_{AB}(x) - u_A
\end{align*}
\]

where \(u\) is the displacement vector of any node on the boundary and the subscript of one letter corresponds to the vertex. The subscripts of the two letters correspond to the edge between the vertices.
where $u$ is the displacement vector of any node on the boundary and the subscript of one particle corresponds to the vertex. The subscripts of the two letters correspond to the edge between the vertices.

The effect of particle orientation on the composite is first analyzed. Figure 3 shows the maximum principal stress and maximum plastic strain inside the composite when doping the same particle shape but with different particle orientations. We find that particle orientation has a significant effect on the stress and strain inside the equilateral triangular particle- and square particle-reinforced composites and a slight effect on the regular pentagonal particle-reinforced composites. We conclude that the higher the internal stress level of the composites, the better the particles enhance the mechanical properties of the composites, and this allows us to determine particle orientation.

### 3.1. Mechanical Parameters Calculation

Figure 4a shows the stress–strain curves of composites doped with different SiCp particle shapes. The stress–strain curves of composites do not vary significantly during the elastic deformation stage. The stress–strain curve of the square particle-reinforced composite has a significant rise during the plastic deformation stage. Figure 4b shows the elastic moduli of composites doped with different SiCp particle shapes, which were obtained by calculation and compared to the elastic modulus of the WE43 matrix alloy (44.2 GPa). The elastic moduli of all kinds of composites are higher than that of the WE43 matrix alloy, indicating that SiCp particle doping provides an enhancement in stiffness for the WE43 magnesium alloy. Moreover, the round particle-reinforced composite has the highest elastic modulus of 52.48 GPa, and the square particle-reinforced composite has the lowest elastic modulus of about 50 GPa.
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The stress–strain curves of composites have no obvious yield stage. Therefore, the stress corresponding to the generation of 0.2% offset strain is used as the nominal yield strength by the panning method. Figure 4c shows the yield strength of composites doped with different SiCp particle shapes as obtained by calculation and compared to the yield strength of WE43 matrix alloy (188 MPa). The yield strength of all kinds of composites is higher than that of the WE43 matrix alloy, indicating that SiCp particle doping provides an enhancement in strength for the WE43 magnesium alloy. Moreover, the round particle-reinforced composite has the lowest yield strength of about 192.2 MPa, and the square particle-reinforced composite has the highest yield strength of about 203 MPa.

Table 2 lists the simulated results of elastic modulus and yield strength for the four models compared to the experimental results. As can be seen, there are errors between the simulation results and the experimental results. The relative error between the average value of the elastic modulus for the four models and the experimental results is 8.6%. The relative error between the average value of yield strength for the four models and the experimental results is 0.36%. The relative error is small, which proves the correctness of the finite element model and the analysis method.

Figure 4. (a) Stress–strain curves, (b) comparison of elastic modulus, (c) comparison of nominal yield strength, (d) comparison of $S_{11}$ and $S_{\text{max}}$.

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Table 2. Comparison of simulation results with experimental results.

| SiCp/WE43 Magnesium Matrix Composite | Elastic Modulus (GPa) | Yield Strength (MPa) |
|-------------------------------------|-----------------------|---------------------|
| Round particle doping               | 52.48                 | 192.2               |
| Equilateral triangle particle doping | 52.28                 | 194.3               |
| Square particle doping               | 50                    | 203                 |
| Regular pentagon particle doping     | 52.31                 | 198                 |
| Average value                       | 51.8                  | 196.9               |
| Experiment result                   | 56.7                  | 196.2               |
| Relative error                      | 8.6%                  | 0.36%               |

3.2. Strengthening Mechanism of SiCp Particles on Composites

Based on the results regarding the characterization of mechanical properties, SiCp particle doping leads to the enhanced strength and stiffness of the composites, and different shapes of SiCp particles have different enhanced effects on the composites. In order to analyze the mechanism behind the effect of particle shape on the mechanical properties of the composites, the distributions of $S_{11}$, $S_{\text{max}}$, and PEEQ inside the composites were extracted separately at the end of the simulation (as shown in Figures 5–7). Figures 5 and 6 show the distributions of $S_{11}$ and $S_{\text{max}}$ for composites with different SiCp particle shapes. The $S_{11}$ and $S_{\text{max}}$ values inside the SiCp particles of each model are higher than those inside the matrix alloy, indicating that although the content of SiCp particles in the composite is low, a larger stress bearing zone is present at the edge of the SiCp particles, which suggests that the SiCp particles undergo a larger load internally that leads to the enhanced strength of the composites. Moreover, the $S_{11}$ and $S_{\text{max}}$ values inside polygonal SiCp particles are higher than those inside round SiCp particles. As a result, polygonal particles provide a better enhancement in the strength of the composites than round particles. When the particle shape is rounder, the enhancing effect on composite strength will decrease. However, in polygonal particle-reinforced composites, the maximum principal stress inside the particle is higher, and the possibility of particle fracture is higher.

The damage is likely to initiate at the interface between the matrix and particle, at the location of the highest stress concentration, as shown in Figure 6. This phenomenon is more prominent in polygonal particle-reinforced composites. Moreover, we found that the $S_{11}$ value at the location of the highest stress concentration is very close to $S_{\text{max}}$, as shown in Figure 4d. Therefore, we initially speculate that the internal damage of the composites under tensile loading along the X-direction is likely to be dominated by $S_{11}$.

Figure 7 shows the distribution of PEEQ for composites with different SiCp particle shapes. The PEEQ inside the SiCp particles of each model are lower than those inside the matrix alloy, indicating that SiCp particles undergo a smaller plastic deformation under tensile loading that leads to the enhanced stiffness of the composites. Moreover, the PEEQ inside round particles is more uniformly distributed and has smaller values than inside polygonal particles. As a result, round particles provide better enhancement in the stiffness of the composite than polygonal particles.
Figure 5. $S_{11}$ distribution of the composite models with different SiCp shapes: (a) round particle doping; (b) equilateral triangle particle doping; (c) square particle doping; and (d) regular pentagon particle doping.

Figure 6. $S_{\text{max}}$ distribution of the composite models with different SiCp shapes: (a) round particle doping; (b) equilateral triangle particle doping; (c) square particle doping; and (d) regular pentagon particle doping.
Figure 7. PEEQ distribution of the composite models with different SiCp shapes: (a) round particle doping; (b) equilateral triangle particle doping; (c) square particle doping; and (d) regular pentagon particle doping.

4. Conclusions

Two-dimensional plane strain unit cell finite element models were established to analyze the potential effect of SiCp particle shape on the mechanical behaviors of SiCp/WE43 magnesium matrix composites. We observed that SiCp particle doping induced an enhancement in the strength and stiffness of the WE43 magnesium alloy because these hard particles underwent a larger load internally and a smaller plastic deformation under tensile loading. Moreover, the damage is likely to initiate at the interface between the matrix and particle, at the location of the highest stress concentration. SiCp particle shape had a strong influence on the mechanical properties of this composite. The polygonal SiCp particles showed a better enhancement in strength, and the square particle had the best enhanced effect on the composite; however, the square particle also exhibited a limited enhancement in stiffness. Moreover, the stress concentrations at the interface are higher and will likely lead to an earlier onset of fracture (and debonding) in polygonal inclusions. As the particle shape became rounder, the enhanced effect on the stiffness of the composite increased.

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