# Influence of particle characteristics on mechanical properties of particle reinforced tungsten alloys

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**Abstract.** The manufacturing processing and the mechanical properties of particle reinforced metal matrix composites are strongly dependent on their microstructural characteristics. In this research, 3D models in microscale of tungsten alloys reinforced by $Zr(Y)O_2$ particles ($W\text{-}Zr(Y)O_2$) were established to investigate their uniaxial compression deformation behaviours. The effects of particles contents, size and their distribution on the compressive properties of $W\text{-}Zr(Y)O_2$ alloy were discussed. The mechanical behaviours of the reinforced W alloys were improved by increasing the content of $Zr(Y)O_2$ particles. With the same particles content, the strength of the reinforced alloys increased with smaller size particles. With the same particle size and content, the stress concentration was reduced with more homogeneous distribution of the reinforced particles. The predicted strengths with 3D models are compared with the experiment data, which exhibits high prediction accuracy.

## Introduction

Particle reinforced metal matrix composites (PRMMCs) show distinct merits over unreinforced metals and alloys, such as high stiffness and strength, outstanding wear resistance, attractive fatigue properties, and superior thermal and electrical characteristics [1, 2]. Designing new PRMMCs and predicting their physical and mechanical performance are challenging. The advanced and reliable numerical models of PRMMCs are essential to optimise and predict their mechanical properties [2, 3].

With the continuous development of numerical methods, the prediction of mechanical properties of materials with simulation has become an important scientific issue [4]. Compared with the traditional experimental methods, the numerical simulation exhibits the following advantages: 1). It is difficult to determine the deformation processing parameters for the materials, such as tungsten, due to their brittleness during the recrystallization. The numerical simulation can predict the mechanical properties over a large temperature range, in which the experimental tests are difficult to carry out; 2). The parameters in numerical simulation could be adjusted easily without the wasting of time and cost; 3). The test conditions, including temperature, duration time and pressure, could be set up smoothly in the numerical simulation. In the past decades, more and more researchers developed the numerical simulation tools to investigate the mechanical properties in room and high temperatures, microstructure evaluation and fracture law of W-based materials.

The mechanical properties of particle reinforced metal matrix composites (PRMMCs) depend on their microstructure characteristics, such as size, fraction, distribution and morphology [3]. The experimental, analytical and numerical simulation methodologies have been employed to investigate the microstructure and physical propriety of PRMMCs. The macroscopic simulation of the composite materials is difficult to reveal the interface evolution, strengthening mechanism and damage. The effective properties and damage mechanism of PRMMCs are strongly dependent on the properties of matrix, particles, interface, and the microstructure of the composites. Various representative finite element models in microscale have been developed to estimate the effects of microstructural features of PRMMCs to optimize their mechanical properties.

The effect of mesoscopic characteristics on mechanical performance of PRMMCs are investigated based on the 2D plane model, which exhibits some disadvantages as follows: 1) the simplified 2D plane model cannot truly characterize actual damage until the whole process of the fracture damage of concrete material and evolutionary regularity of crack extension; 2) it cannot accurately reflect the macroscopic mechanical properties of PRMMCs. In the actual production and life, the mechanical problems and the structure of the composite materials relate to dimensional entities. It is necessary to establish a 3D numerical model to study the mechanical properties and failure mechanism of PRMMCs more truly and intuitively. 3D model has been proposed to analyze the influence of particle size [5], volume fraction [6], morphology [7], distribution [8], interface damage [9], crack and void evolution [10] on the mechanical performance of composite [8, 9, 11]. Compared with 2D model, 3D model is more realistic in the characterization of the microstructure.

Zhang et al. [7] investigated the effects of particles' aspect ratio on the deformation of Al-SiC composite by using microscale models. The representative volume element-based microscale model of the composites with different particle aspect ratio was employed. An elastoplastic model was employed to describe the relation between the stress and the plastic strain of the Al matrix [12]. The simulation results show that in the longitudinal direction, the stress in the SiC particles increases with their aspect ratio and the stress in the metal decreases. The effects of the particles' shape and size on the mechanical properties of the reinforced composites are essential to achieve the numerical simulation with W alloys. Williams et al. [11] studied the effects of particle and matrix interface debonding in Al-SiC composites. Different microstructures containing angular and idealized ellipsoidal SiC particles were analyzed. During plastic deformation, an isotropic matrix hardening model was introduced to describe their mechanical behaviour. The results indicated that the angular particles exhibit higher degree of load transfer and are more sensitive to interfacial debonding during tensile deformation. The geometrical shape of the reinforced particles is important to investigate the improvement of the mechanical property of the reinforced alloys.

In this study, the microscale model of particles reinforced tungsten alloy is established. The complete stress-strain field in microscale of PRMMCs is obtained to reflect their mechanical characteristics. The influence of material parameters such as $Zr(Y)O_2$ particle contents, size and distribution on the mechanical properties of W alloy is investigated, which may be necessary for the mechanical design of structural materials in computational materials science.

This paper is structured as follows: In Section 2, manufacturing processes are presented for the elaboration of W-$Zr(Y)O_2$ alloy. In section 3, 3D simulation model is introduced with the associated boundary conditions. Section 4 consists the numerical simulation results. A comparison with experimental investigations is conducted in Section 5. The main conclusions were summarized in Section 6.

## Presentation of W-$Zr(Y)O_2$ alloys

Four kinds of doped tungsten powders, 0 wt% $Zr(Y)O_2$, 0.25 wt% $Zr(Y)O_2$, 0.5 wt% $Zr(Y)O_2$, and 0.75 wt% $Zr(Y)O_2$, have been used in this study. The manufacturing processes concerning the fabrication of W-$Zr(Y)O_2$ alloys was described as follows [13]: Firstly, $ZrOCl_2 \cdot 8H_2O$, $Y(NO_3)_3 \cdot 6H_2O$ and $(NH_4)_6H_2W_{12}O_{40} \cdot 5H_2O$ were dissolved in distilled water. A certain amount of $ZrOCl_2 \cdot 8H_2O$ and $Y(NO_3)_3 \cdot 6H_2O$ were homogeneously mixed. The mixture was added slowly to the $(NH_4)_6H_2W_{12}O_{40} \cdot 5H_2O$ solution with stirring. $HNO_3$ was adopt to decrease the solution's pH value to lower than 1.0. The mixed solution was put into a stainless-steel autoclave with a polytetrafluoroethylene lining. The autoclave was sealed and then heated at 276.5 K min$^{-1}$ until the reaction temperature was reached to 120°C. The holding time of the hydrothermal reaction was 17 h. The product was stirred for 120 min using an electric mixer with some distilled water. Through drying at 90°C, the precursor powder was obtained. The obtained powder was calcined at 550°C for 4 h in air and reduced through the hydrogen reduction processes 550°C (2 h) + 900°C (2 h). The milled powders were pressed by the cold isostatic pressing process at a pressure of 250 MPa. The green compacts were sintered at 2400°C for 4 h in a hydrogen atmosphere. Then the sintering samples were hot isostatic pressed at 1400°C and 200 MPa for 1h. Over 90% of particles range from 100 nm to 650 nm in diameter without the coarse particle of more than 1 μm. The average particle size is about 410 nm.

## Numerical simulation in 3D microscale of W-Zr(Y)O2 alloy

3D model is representative of the experimental compression specimen, with the size of 5×8 μm. In the numerical simulation, it is assumed that all $Zr(Y)O_2$ particles in W matrix are homogenous and considered as spherical with a constant diameter, which is calculated based on their volume fraction. The coordinates of the particles were generated by using the random distribution function. They should satisfy two conditions: firstly, the particles should not exceed the boundary of the model, it means that the radius of particles should be smaller than the distance between the center of particle and the boundary; Secondly, the particles cannot overlap with each other.

The matrix and particles are merged together in the numerical model. The contact conditions between the matrix and circles are not considering in the simulation. The lower and upper mold tools are created as rigid body in the numerical model: one is placed on the top surface of the W alloy and the other one is placed on its bottom surface. The lower tool is fixed, while an imposed displacement of 1.3 μm is applied on the upper tool. The imposed displacement is calculated according to the sample height and strain in the experimental tests. The friction between the tools and W alloy is not considered in the simulation. The top and bottom surfaces of the W alloy are free to move in radial direction. The 3D cylindrical geometry model is 5 μm in diameter and 8 μm in height. The tetrahedral element C3D10 is used in the modelling.

## Simulation results of compression tests with W-Zr(Y)O2 alloy

Validation of mesh size. In order to improve the calculation accuracy of the numerical simulation, different mesh conditions are applied on the 3D model. The mesh size, including 0.3 μm, 0.4 μm, 0.6 μm and 0.8 μm, corresponding to element number of 777915, 138712, 93730 and 79978 are employed in the simulation, as shown in Fig. 1.

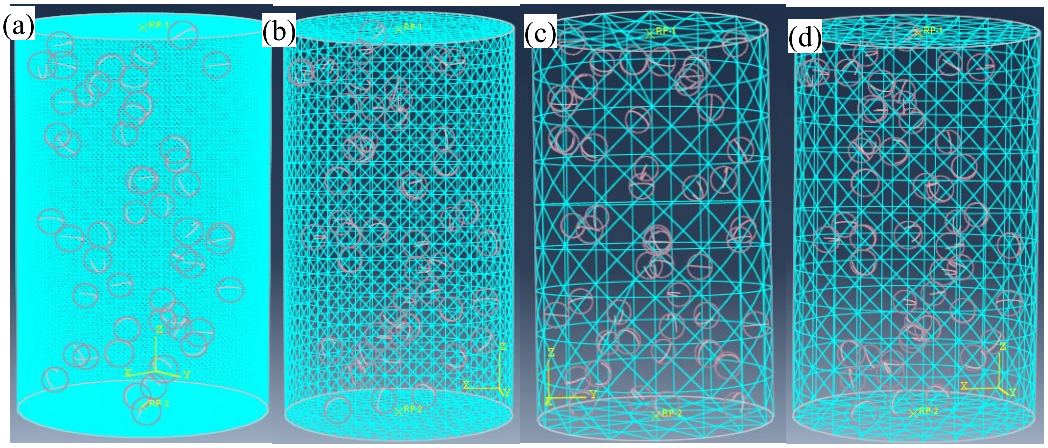

*Fig.1. 3D models with different mesh size: (a) 0.3 μm; (b) 0.4 μm; (c) 0.6 μm; (d) 0.8 μm.*

The 3D models with different mesh size are created in the simulation to study the convergence of mesh. The evolution of stress in function of mesh size is illustrated in Fig. 2. The stress decreased with the mesh size and becomes constant until mesh size 0.3 μm. The mesh size 0.3 μm is selected to achieve a high calculate accuracy with reasonable computational time.

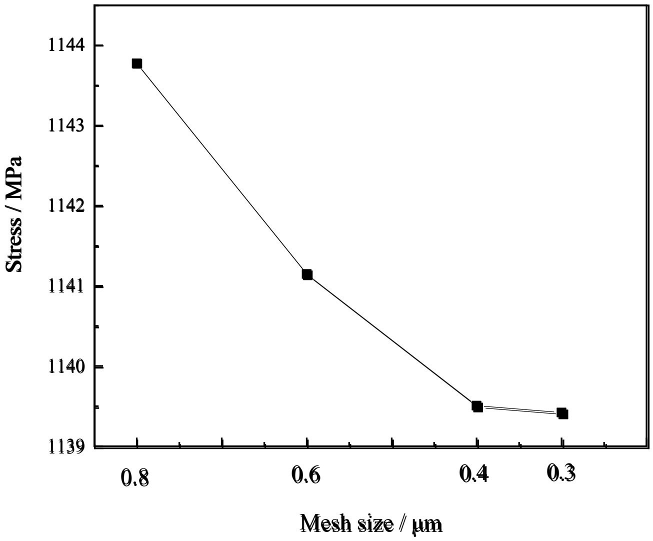

*Fig. 2. Evolution of the von Mises stress in function of mesh size.*

$Zr(Y)O_2$ mass fraction. The mass fraction of $Zr(Y)O_2$ has a significant effect on the mechanical properties of reinforced W alloy. The effects of particle mass fraction on mechanical behaviors, including yield and compressive strength, are calculated by using the 3D model. 3D model with different particle mass fraction are created as shown in Fig. 3. The particle number in each model is 50.

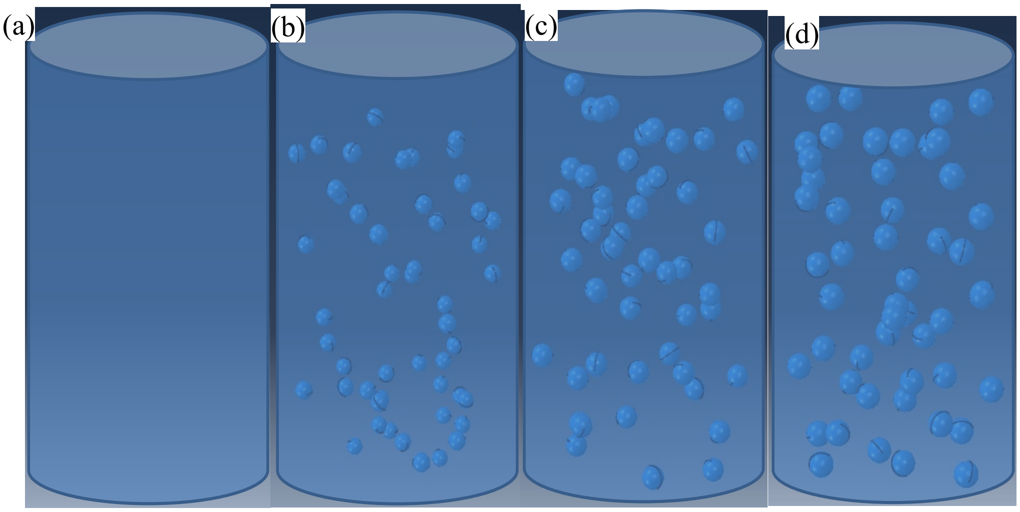

*Fig. 3. 3D models embedded with 50 particles with different mass fraction of $Zr(Y)O_2$: (a) 0; (b) 0.25 wt. %; (c) 0.50 wt. %; (d) 0.75 wt. %.*

Based on Fig. 4a, the ultimate compressive stresses obtained by 3D models increase slightly with the particle mass fraction. Fig. 4b shows that, when the particle mass fraction increases from 0 to 0.75 %, the ultimate compressive stress of the material increases from 1117.7 MPa to 1140.1 MPa, which is 2.77 % higher than that of the undoped alloy. When the particle mass fraction increases from 0 to 0.75 %, the yield strength increases 3.91 %. Fig. 5 presents the stress distribution of axial section in loading direction of 3D models. As the particles randomly distributed in the whole 3D model, a small number of visible particles are in the whole 3D model compared to corresponding 2D model. As the mass fraction of particle increases, the maximum stress in loading direction observed does not vary linearly. This is attributed to the various particle number existed in or near axial section in different models. This comparison shows the stress in the matrix increases with particle content. It indicates the reinforcement effect of particle on the matrix.

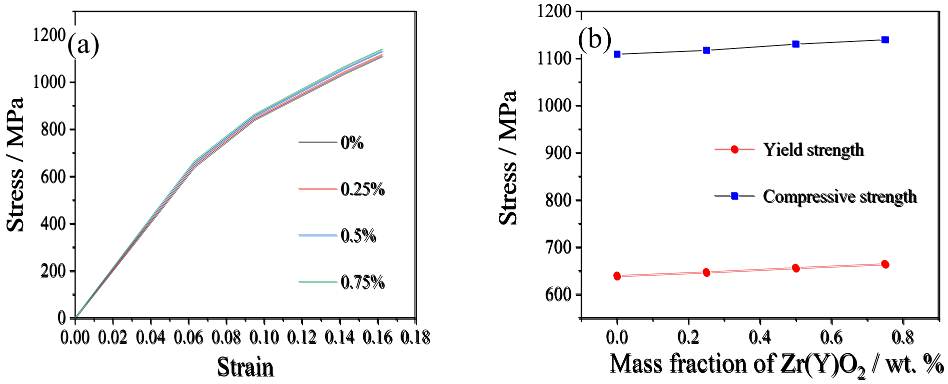

*Fig. 4. Mechanical properties obtained by 3D models with different particle mass fraction: (a) Stress-strain curves; (b) Yield and compressive strength.*

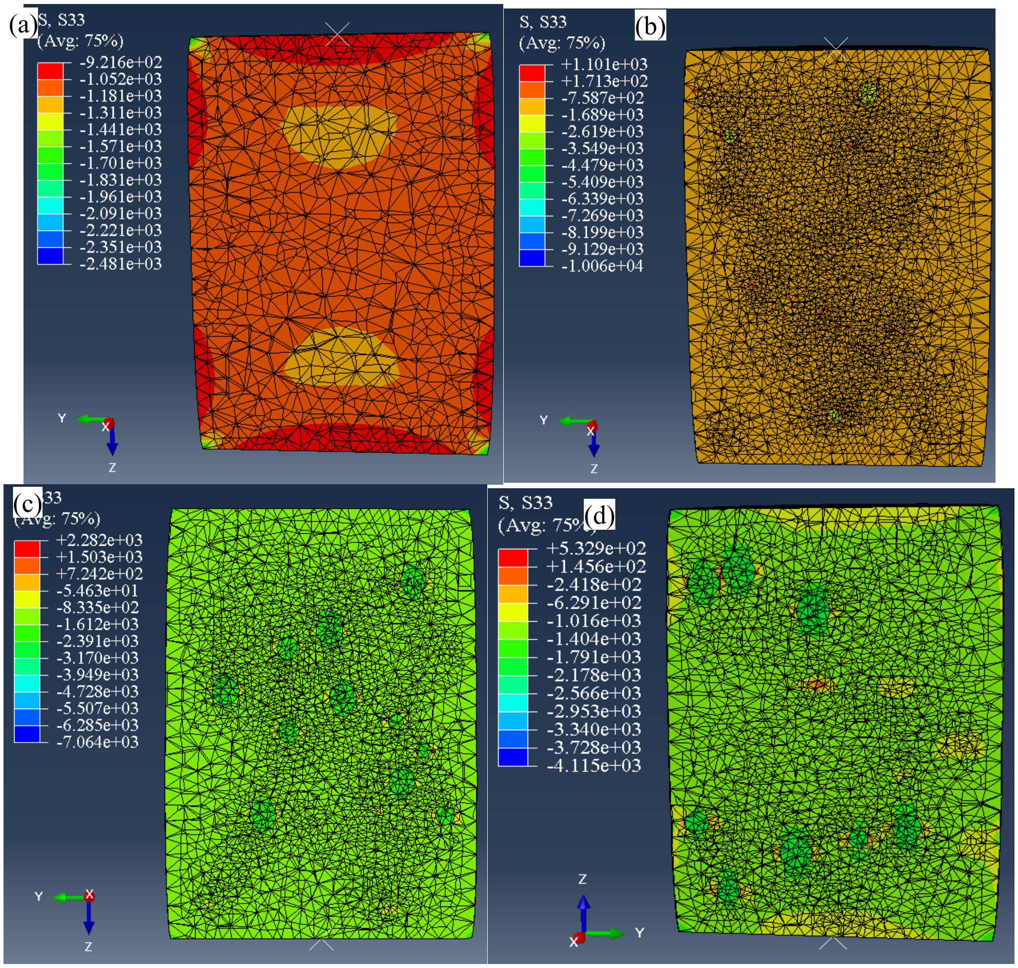

*Fig. 5. Stress distribution in loading direction of 3D models embedded with 50 particles with different mass fraction of $Zr(Y)O_2$: (a) 0; (b) 0.25 wt. %; (c) 0.50 wt. %; (d) 0.75 wt.*

## Comparison of simulation results with experimental investigations

The mass fraction of the particles in the two models affects the yield strength. The simulated values are compared with the experimental values of the room-temperature compressive properties of W-Zr(Y)O2 alloy by HIP. The yield strength of the reinforced alloys increases with the mass fraction of the particles, both in the numerical simulation and experimental investigation, as shown in Fig. 6. The numerical results in the 3D simulation are more important than these in the 2D simulation and closer to the experimental data. The difference between the numerical and experimental results is mainly due to no consideration of the interaction conditions between particles and matrix, and the grain refinement in the alloys.

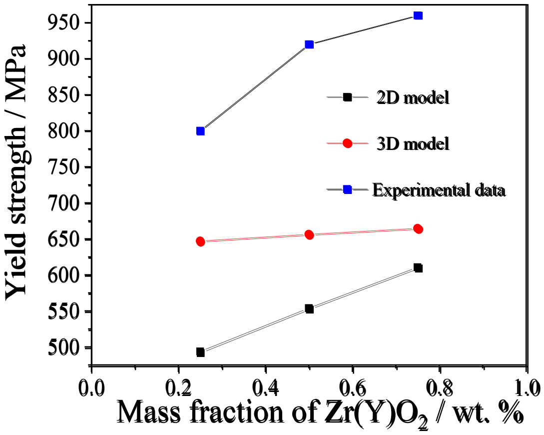

*Fig. 6. Effect of Zr(Y)O2 mass fraction on yield strength of reinforced alloy in numerical models and experimental investigations.*

## Conclusions

1. The random distribution of particles in W matrix is generated and implemented with finite element software Abaqus.
2. 3D models in microscale are created by considering of the material properties of W-Zr(Y)O2. The influences of the particle mass fraction on their behaviours are investigated. The yield increases by 3.91 % when the particle mass fraction increases from 0 to 0.75 %. The predicted strengths from 3D simulation are higher than those from experiment data.
3. The proposed numerical approach will be employed to develop the innovative particle reinforced materials with high performance at various temperatures. The simulation models enlarge its applications for other solicitations, such as tensile, shear and torsion.

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