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MECHANICAL FINITE ELEMENT ANALYSIS OF TUNGSTEN ALLOYS USING MULTI-PARTICLE UNIT CELL MODELS

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ABSTRACT

Multi-particle unit cell models containing some important microstructure characteristics of particle reinforced metal matrix composites (91%wt tungsten alloys) were established to study the mechanical properties and the fracture patterns of the alloys under tensile loadings. A new fixed point iteration method for multi-particle unit cell's boundary condition was presented to provide the displacement constraint conditions for the multi-particle unit cell models. The effects of tungsten content, particle shape, particle size, and interface strength on the mechanical properties of tungsten alloys were analyzed. The relationship between the mechanical behaviors and the microstructure parameters was studied. Based on the comparison of the experimental results and the numerical predictions, a good agreement between them is obtained, indicating the rationality of the fixed point iteration method in FE analysis of particulate-reinforced metal matrix composites.

***Keywords*:** multi-particle unit cell model, fixed point iteration method, fracture behavior, particulate-reinforced composites, microstructure.

1. INTRODUCTION

Tungsten alloys possess high density, strength, and ductility, which makes them useful for military and civilian applications. The composite microstructure consists of nearly spherical grains of body-centered cubic tungsten surrounded by a solidified face-centered cubic matrix phase containing Ni, Fe. The two-phase composite structure of tungsten alloy determines that the macroscopic deformation and fracture behavior have close relation with the microstructure of the composites. Therefore, it is important to investigate the relationship between the microstructure and the mechanical properties of the composites under different loadings, which provides practical values for the improvement of the mechanical properties and the optimization of tungsten alloys [1-4].

By using a compression Kolsky bar, Coates and Ramesh [5] investigated the deformation of a liquid-phase-sintered W-Ni-Fe heavy alloy. They found that the compressive flow stress of this tungsten heavy alloy increases with the increasing of strain rates from $10^{-4}s^{-1}$ up to about 7.0×10^3 s^{-1}. Kim *et al.* [6] studied the effect of the size and shape of tungsten particles on dynamic torsional properties in tungsten heavy alloys and reported that the size of tungsten particles and their hardness were increased as sintering temperature and time were increased and there would be an appropriate tungsten particle size because the cleavage fracture mode would be beneficial for the "self-sharpening" of the tungsten heavy alloys. Song and Ning[7] investigated the mechanical characteristics and the fracture behavior of tungsten alloys 91W-6.3Ni-2.7Fe by in-situ tensile tests and numerical simulations and the crack propagation in the composites was examined.

With fast development of computers, numerical simulations have been gradually accepted by scientists worldwide [8-9]. Preferred over physical experiments, numerical simulations draw more attraction due to their low cost, easy setting of parameters, and high repeatability. Böhm *et al.* [10] employed a multi-inclusion unit cell models to study the effects of the reinforcements types and shapes and analyzed the predicted microfields in terms of their phase averages and the corresponding standard deviations. Tang [11] studied the fracture process of high particle reinforced

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composites with under tensile loading. The deformation, the initiation and the propagation, and the interaction between the particles of cracks in the composites were discussed in detail. Bao and Ramesh [12] presented the stress-strain curves of 80 wt % and 94wt% tungsten alloys under uniaxial compression by adopting three kind of element model and found the stress-strain had no relation with the particle size.

In these literatures, boundary conditions for the models are periodical boundary conditions, kind of artificial boundary conditions. Using these boundary conditions may lead to some errors in numerical simulations. In the current paper, a new method for the real boundary conditions is presented.

2. FIXED POINT ITERATION METHOD FOR BOUNDARY CONDITIONS

The problem of solving the effective mechanical parameters of composites with periodic microstructure can be considered to solve a nonlinear functional equation $\Phi(\xi_m, \xi_p, f, u, \xi) = 0$. ξ_m and ξ_p are the mechanical parameters of the matrix and the reinforcement, respectively. ξ is the effective mechanical parameter of the composite. As it is known, the solution for $\Phi(\xi_m, \xi_p, f, u, \xi) = 0$ exits and has a single value. According to Banach[13]fixed point theorem, the fixed point ξ can be obtained by repeated iteration, only when a initial value ξ_0 and a compression mapping are found on the basis of $\Phi(\xi_m, \xi_p, f, u, \xi) = 0$.

2.1. Determining the Initial Value of ξ_0

Based on Banach fixed point theorem [13], the fixed point ξ can be found by repeated iteration no matter how the initial value of ξ_0 is chosen, only when T is a compression mapping. The step number of iteration becomes more and more smller when the initial value of ξ_0 approaches. In present study, the mechanical parameter ξ_m is chosen as ξ_0.

2.2. Determining the Compression Mapping *T*

The compression mapping can be divided into two sub-steps:

(1) Microscopic to macroscopic: The boundary value problem of macroscopic field is solved by using the effective mechanical parameter obtained from the *i* th iteration as an input condition. Then, the boundary conditions for next step can be obtained from the calculating results. This process is defined as T_{B2W} and $\Gamma_{i+1} = T_{\mathrm{B2W}}\, \xi_i$, where Γ_{i+1} is the boundary condition of the unit cell in the $i + 1$ th iteration.

(2) Macroscopic to Microscopic: Pick up the boundary conditions from the calculating results of the boundary value problem of the macroscopic field. By using the above boundary conditions, the effective mechanical parameter ξ_i can be obtained by solving the boundary value problem of the microscopic field. This process is called $\mathrm{T_{W2B}}$ and $\xi \mathrm{i} = \mathrm{T_{W2B}}\, \Gamma_i$.

3. FINITE ELEMENT MODELLING AND NUMERICAL SIMULATIONS

Consider the microstructure of composites as the periodic and repeating array of a heterogeneous unit cell. In Fig. 1, a macroscopic homogeneous model is established by using $\xi_0 = \xi_{\mathrm{m}}$. The freedom of the left end of the model is constrained and on the right end, uniform tensile load is applied. An area, having the same size with a unit cell, is chosen. The displacement values of all the nodes on the boundary in the area are picked up from the calculating results. In Fig. 2, a multi-particle unit cell model is established by applying the displacement values on the corresponding nodes (the black points). The displacement boundary conditions for the other nodes are gained by the linear interpolation of the known nodes. The next step is to solve the boundary value problem. The effective mechanical parameter ξ_1 can be obtained on the basis of the $\sigma_e - \varepsilon_e$ curve plotted by the numerical results. Then, establishing another macroscopic homogeneous model by using ξ_1 and the rest may be deduced by analogy until $\xi_{n+1} - \xi_n \le \varepsilon$ (ε is a small quantity) ξ_n is the solution of $\Phi(\xi_1, \xi_2, f, u, \xi) = 0$ and also is the effective mechanical parameter of the composites. The boundary condition Γ_n presents the real movement of the boundaries of the unit cell in the composite under simple tension.

3.1. Material Model and Material Parameters

Plastic kinematic material models were adopted for both the tungsten particle (W particle) and the matrix. Element 2D solid 162 are chosen for both the reinforcement and the matrix. Table.1 lists the material parameters used in numerical simulations. All the parameters were determined by experiments.

Table 1
Parameters used in Numerical Simulations

	Density $\rho(g/cm^3)$	*Young's modulus* $E(GPa)$	*Poisson's ratio* μ	*Yielding stress* $\sigma_y(MPa)$	*Tangent modulus* $E_t(MPa)$
Tungsten particle	19	410	0.27	800	500
Matrix	15	200	0.31	300	150

3.2. Numerical Predictions and Experimental Results

Numerical simulation was performed to investigate the mechanical properties of tungsten alloys under tensile loading. The stress-strain curves obtained from the simulation was compared with that of the experiments.

Seen from Fig. 3, there is a good agreement between the numerical predictions and the experimental results. Some differences of Young's modulus were found in elastic stage. There are two reasons for the deterioration in elastic modulus:

(1) The materials are considered as ideal materials without any microdefects and the tungsten-matrix interfaces are perfect in simulations.

(2) W particle is circular or elliptical with the same size and is uniformly distributed in FE model, while in experiments, W particle is randomly distributed and the particle size is different.

Based on the comparison, it is concluded that the fixed point iteration method can be used to analyze the mechanical properties of particle reinforced metal matrix composite. The FE model can be adopted to investigate the effects of microstructure parameters on the macroscopic mechanical properties. In present study, four different tungsten contents were considered in numerical simulations, such as 85%, 88%, 91%, and 94% (mass fraction). Fig. 4 presents the unit cell of four different tungsten contents. From Fig. 12, the elements are nearly uniform and have approximately the same size.

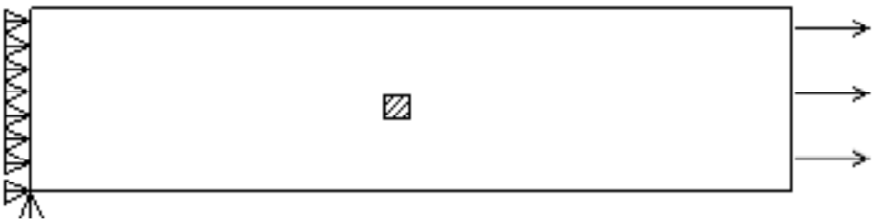

Figure 1: Homogenous Material Model

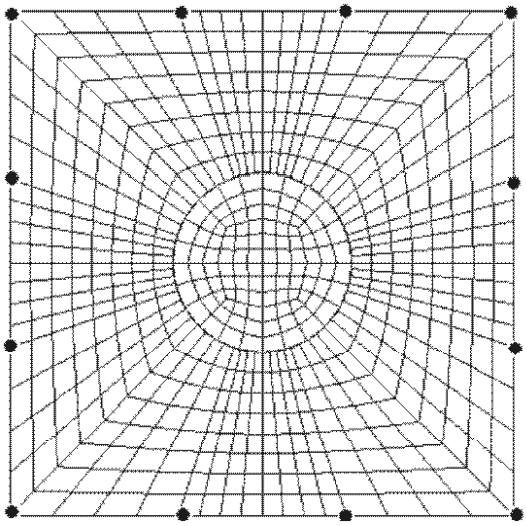

Figure 2: Finite Element Model of Unit Cell

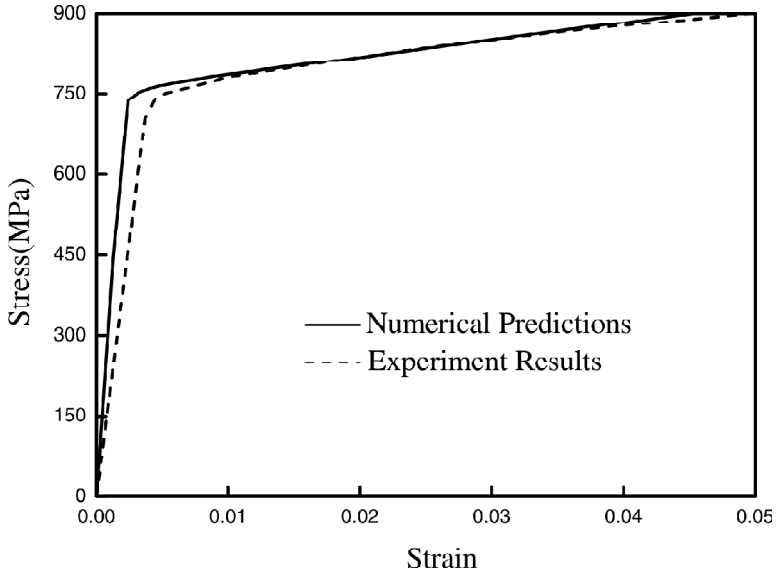

Figure 3: Comparison of Experimental Results with Numerical Predictions

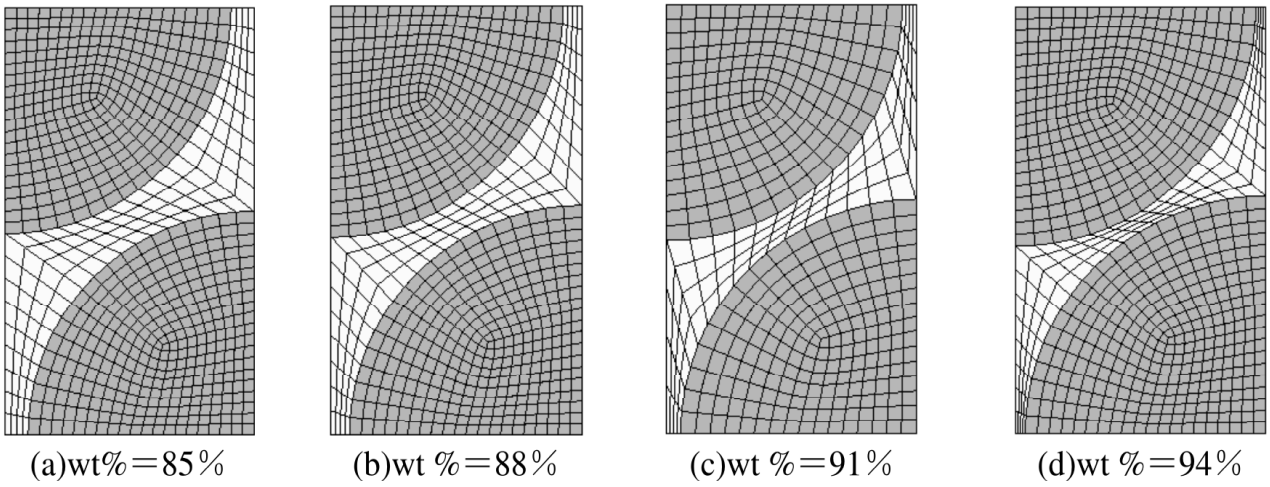

Figure 4: The Unit Cells for Different Contents

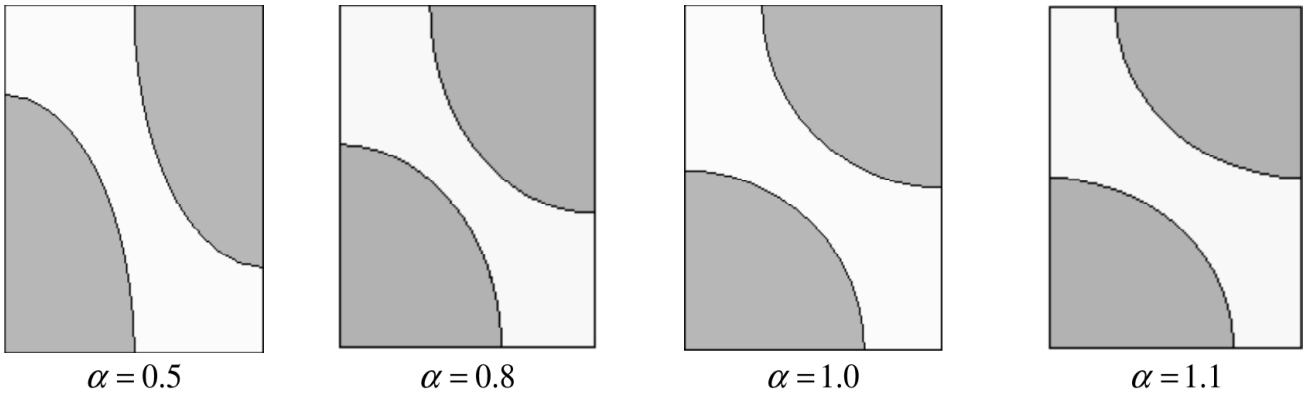

Figure 5: The Unit Cells for Different Aspect Ratios

Four different aspect ratios ($\alpha = l / d$, ratio of major axis/minor axis of tungsten particles), such as 0.5, 0.8, 1.0, 1.1 were used to establish the unit cell, simulating different particle shapes.

The multi-particle unit cell is established by copying the unit cell in the longitudinal direction and the transverse direction. Fig. 6(a) is the unit cell of 85 wt % tungsten alloys. The geometry size of the multi-particle is 19μm × 11μm in length and width. Fig. 6(b) is the unit cell of tungsten alloys ($\alpha = 0.5$). The length and the width of the multi-particle are 16μm and 12μm, respectively. All numerical simulations are performed on the multi-particle unit cell, when the boundary conditions are exerted by the fix point iteration method.

The influence of tungsten content on tensile properties is demonstrated in Fig. 15. From Fig. 7, it can be seen that increasing tungsten content from 85wt% to 94 wt% results in an increase in yield stress about 50MPa.

Fig. 8 shows the effect of variation in tungsten particle shape on the tensile behavior of tungsten alloys. The aspect ratio has little effect on the tensile properties of tungsten alloys without considering the forging deformation of tungsten particle. Forging process can improve the yield stress and strength of tungsten alloy, which will results in a decrease in the elongation of the material and a shape change of tungsten particle.

In order to simulate the failure of tungsten-matrix interfaces, these interfaces are divided into ideal interfaces and non-ideal interfaces by the setting of CONSTRAINED_TIE-BREAK, one of the constrain type of LS-Dyna. Tie-breaks may be used to simulate the effect of failure along a predetermined line, such as a seam or structural joint. When the failure criterion is reached in the adjoining elements, nodes along the slideline will begin to separate. As this effect propagates, the tie-breaks will appear to“unzip,” thus simulating failure of the connection. Series of cases were performed to simulate the propagation of the cracks according to the two different interfaces.

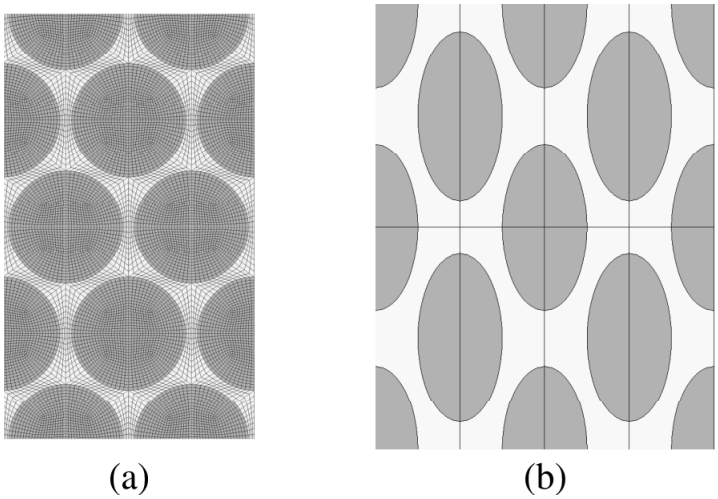

Figure 6: The Multi-particle Unit Cell

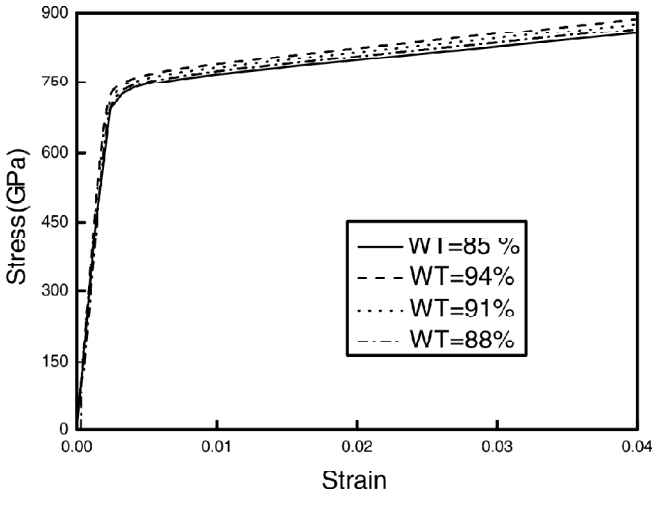

Figure 7: Effect of Variation in Tungsten Content on the Tensile Behavior of Tungsten Alloys

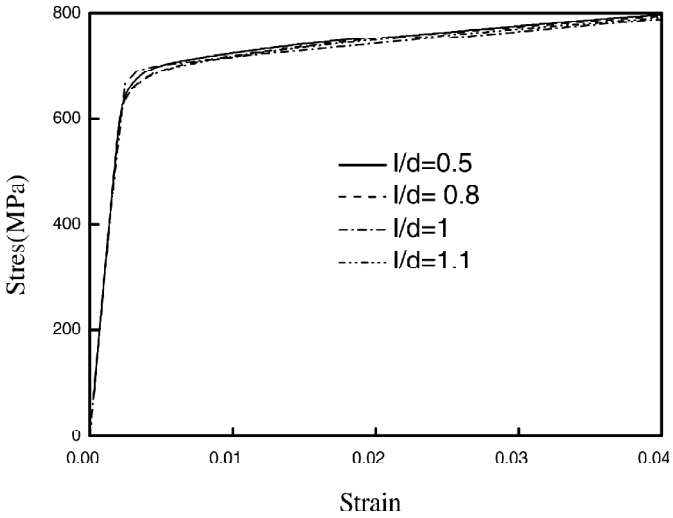

Figure 8: Effect of Variation in Tungsten Particle Shape on the Tensile Behavior of Tungsten Alloys

4. CONCLUSIONS

Numerical simulations were carried out to investigate the mechanical properties and the fracture behavior of 91W-6.3Ni-2.7Fe tungsten alloys. Fixed point iteration method was presented for unit cell's boundary condition. By adopting the method, finite element (FE) models of unit cell was established. Series of cases were performed to explore the influence of the microstructure characteristics on the mechanical properties of tungsten alloys and the typical fracture patterns of tungsten alloys under tensile loading were simulated. It was found that increasing tungsten content resulted in an increase in yield stress and the particle shape had little effect on the tensile properties of tungsten alloys. Interface strength of tungsten-matrix had a relatively strong contribution to the fracture patterns of the composites. Comparison of the experimental results and the numerical predictions shows a good agreement between them, which verifying the rationality of the FE models based on fixed point iteration method.

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