Finite Element Modeling of Properties Influence of Particle Characteristics in Particle Reinforced Metal Matrix Composite

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Properties Influence of Particle Characteristics in Composite

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ABSTRACT

The characteristics of particle reinforcement have significant impact on the performance improvement of particle-reinforced composites, which include particle size distribution, shape, volume fraction and the nature of the interface. A model of a two-dimensional randomly distributed spheroidal particles coupled with an axisymmetric unit cell model containing one reinforcing particle with a transition interface was proposed. Macroscopic mechanical properties were simulated with the two-dimensional randomly distributed spheroidal particles model and the effects of interface characteristics were discussed in the single reinforcing particle axisymmetric unit cell micro-model. This micro-model is developed considering the supposed impact of the interface compatibility between the reinforcements and the matrix. The

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influence of interfaces on the composite modulus and the stress-strain distribution was discussed with this model. It was shown that composites with transition interfaces could bear higher stresses than those with simple zero-thickness interfaces.

Keywords: computer simulations; metal matrix composites; mechanical properties; surfaces and interfaces; intermetallics; elasticity

1. INTRODUCTION

The particles adopted are usually non-metallic such as ceramics and graphite, as they tend to have such properties by their own. The main factors to be considered when choosing a type of particle should include shape and size, physical properties, mechanical properties, processing and its compatibility with the matrix. The currently widely used particle reinforcements are SiC, BC, and Al_2O_3, which are effective in increasing composite strength and modulus. However, the drawback is the significant loss of ductility. The ceramic particles are brittle materials. Under stress, the particles themselves, and the particle-particle and the particle-matrix interfaces can all fracture, leading to the composite failure.

A new Mg–Li matrix composite with 5 wt.% YAl_2 particulates was developed by stir-casting technique [1]. Its microstructures and properties were investigated systematically. The results show that the YAl_2 intermetallics particles distribute in Mg–Li matrix homogeneously, and a good YAl_{2p}/Mg–Li interface is developed wherein there are no reaction products or obvious elements diffusing. The composite has a higher tensile strength compared with matrix alloy, whose good ductility is kept.

It has been found that the intermetallic YAl_2 when used as particle reinforcement can be beneficial to the composite ductility while at the same time effectively increasing composite strength. Microscopy showed good interface connection between the reinforcing particle and the matrix, without voids, interface fracture, interface reaction, and amorphous layer formation. These all contribute to the better composite properties.

In order to identify the mechanisms of particle reinforcement in metal matrix composites, we need to consider the following two aspects when setting up models:

(1) The distribution and shape of the particles in the model must be representative of the real composite material. The size of the model should be as large as possible to reduce boundary effects.

(2) A true reflection of the particle reinforcing effect, especially in terms of the good interface between particles and matrix as observed experimentally. The model needs to describe and simulate such interface correctly.

In the past, many researchers have designed axisymmetrical unit cell models containing one reinforcing particle [2], spheroidal unit cell model incorporating interactions between particles [3], cubic model of randomly distributed spherical particles [4], and cell model containing interface [5] using the serial sectioning method [6,7]. These models can simulate to a certain extent the tensile and fracture behaviour of particle reinforced metal matrix composite materials. Using these models, the effects of reinforcing particle volume fraction, shape, size, and interface on the mechanical properties of the composite materials have been analysed. Some results have emerged. For example, it has been found that smaller reinforcing particles are more effective in improving properties of composite materials and minimising failure of the materials [8]. Circular and smooth reinforcing particles reduce stress concentration in materials and thus minimise fracture at the interface [9]. Also, it has been found that uniform particle distribution is beneficial to homogeneous stress and strain distribution during the material deformation process, thus avoiding local stress concentration [10,11].

All the existing models, while solving some problems, have their limitations. Examples of these are the assumption of periodicity of particle distribution, the assumption of spherical particles, the difficulty in software manipulation, and the lack of universal applicability of the software. In addition, there is some way to achieving a comprehensive theoretical framework, capable of evaluating all relevant factors. Therefore, constructing more realistic micro-scale models of particle reinforced metal matrix composites, representing real material conditions and with universal software applicability, is an important and immediate task. Such models will help exploring the effects of various factors on the composite material properties, and directing the future research and development of new composite material systems.

An interface transition region can be formed through the following ways:

(1) Chemical reaction at the interface between the reinforcing body and the matrix;

(2) Coating on the reinforcing body;

(3) Diffusion of elements across the interface;

(4) Even the mechanical interface, where the reinforcing body and the matrix are mounted mechanically at the interface, will have finite thickness with varying bonding strength across the interface thickness.

Considers the effect of particle shape, distribution, volume fraction and interface, this paper proposes a two-dimensional model of randomly distributed spheroidal particles [12] coupled with an axisymmetric unit cell model containing one reinforcing particle. The aim is to develop a platform for further coupled computation based on micro as well as macro models for simulating micro phenomena as well as experimental validation of composite materials.

It is well known that the physical and mechanical properties of metal matrix composites are strongly dependent on the characteristics, size and number distribution of the reinforcing particles, but we will now explain why the interface strength between the matrix and the reinforcing particles is as important. One of the main reasons of the significantly increased strength of a metal matrix composite over the metal matrix is that the reinforcing phase can take part of the load on the composite. The load transfer from the matrix to the reinforcing body is through the interface between them, and therefore the strengthening mechanisms are strongly related to the strength of the interface. A good interface with good connection and high interface strength can transfer the load effectively, and help increase the composite strength. Conversely, a poorly connected interface will not be ideal for strengthening.

Therefore, the interface quality determines the efficiency of the load transfer from the matrix to the reinforcing body. There are several types of interface connection in composite materials:

(1) Simple connection interface, without solution, diffusion, reaction and having good wettability. This is a clean and tight-bonding interface. Semi-coherent atom-matching interface belongs to this type of interface.

(2) Solution or diffusion interface. As the name implies, there is interdiffusion between atoms in the reinforcing particles and the matrix in the interface region.

(3) Reactive interface, due to the formation of new chemical compound(s) through chemical reactions at the interface.

(4) Mechanical interface. The reinforcing body and the matrix are mounted mechanically at the interface. Rougher interfaces are beneficial to such mechanically connected interface by making the bonding stronger.

If the interface strength is weak, it will directly affect the strength of the composite system. Under stress conditions, defects usually initiate at the weak interface. Part of this paper will describe the unit cell model containing one interface layer and examine the effect of the elastic modulus and the yield strength of this single layer on the stress and strain distributions in the composite material. Finally, the discussion will be extended to interfaces with several transition layers forming a gradient of properties.

2. THE PROPOSAL OF COUPLED MODEL OF PARTICLE REINFORCED METAL MATRIX COMPOSITES

The models in the past were mostly unit cell models having various shapes [4]. Randomly distributed spherical particles were usually considered. Upon applying external stress, the internal stress distribution can be calculated. In reality, however, the particles in a composite material would not be periodically distributed as often assumed in unit cell models. In addition, affected by processing, the particle shape is not necessarily spherical, but is more likely spheroidal. In the present programme of work, we have established a randomly distributed spheroidal particle model (Fig. 1) [12]. Based on literature and experimental data and cross validation, the effects of particle material parameters, geometrical parameters and volume fractions on the composite tensile properties are discussed in a recently published paper [12].

During experiments using the intermetallic YAl_2 as particle reinforcement, it was found that the good interface connection between this kind of reinforcement and the matrix is possibly the reason for maintaining a good level of ductility whilst increasing the modulus and strength. Based on this finding, we have set up a unit cell model including interface layers, in order to investigate the effect of the interface elastic modulus and the interface strength on the composite material. The objective was to set up a model describing the interface transition layer. Therefore, combining the models described in [12] and in the following sections of this paper, we will be able to obtain a coupled model describing the entire particle reinforced metal matrix composite structure (Fig. 2). The key concept in the model focused next in this paper is the expression of the interface transition layer, enabling simulating the effects of gradual, i.e., not sharp interface between the particle and the matrix.

The macro and micro models are based on the same reinforcing particles and the matrix material, but with different shape and distribution. The material parameters are given in Ref. [12]. When not considering fracture, the main material phenomena under external stress are elastic and plastic deformation, and thus the elastic modulus and the yield strength are the main parameters. In Ref. [13], we have described the model used for simulation in sections below.

3. MODEL WITH ONE INTERFACE LAYER AND THE EFFECTS OF ITS MODULUS AND STRENGTH

This section will start the simulation and discussion of the effects of the interface layers on composite properties, and build a foundation for further investigation of such effects. The aim is to set up a transition interface and evaluate the necessity and effectiveness of using the transition interface in modelling. To achieve this, we first use a unit cell model, apply a uniaxial stress, and calculate the stress and strain in the composite for varying elastic modulus and yield strength of one transition interface layer.

As there is no experimental data available for the material parameters of the interface layer, we make an assumption that this layer has properties in between the matrix and reinforcing body, when the interface bonding is good. With this assumption, the base material parameters adopted in modelling are listed in Table 1, where the interface parameters are around averages of data from the matrix and the reinforcement.

3.1. Effect of Interface Elastic Modulus on Composite Properties

The calculations in this section use the base material parameters as shown in Table 1, except that the interface elastic modulus is varied above and below the base value of 100 GPa. With varying elastic modulus of the interface layer, under a fixed load of 100 MPa that is slightly larger than the matrix yield strength, the maximum stress of the interface and the maximum stress within the composite system are given in Table 2. It can be seen that when the interface modulus is lower than 100 GPa, the interface maximum stress does not change a great deal, and remain slightly lower than the maximum stress within the composite system. However, the stress taken by the interface is always greater than the average applied stress, i.e., load. Therefore, when the interface has a high yield strength, of 1000 MPa, it having a low elastic modulus does not affect the composite properties much.

When the interface modulus is greater than 150 GPa, i.e., greater than the reinforcing body's modulus, the maximum stress in the entire composite system occurs at the interface. Fig. 3 shows the internal stress distribution in the composite system when the interface elastic modulus is 1000 GPa. It can be seen that the interface undertakes the largest stress. This is detrimental to the composite when the interface strength is not very high. Therefore, the modelling shows that the elastic modulus of the interface is significant to the performance of the composite.

Next, we change the loading to 80 MPa, i.e., just below the matrix yield strength, and 120 MPa, i.e., just above the matrix yield strength, and examine the trend of change in the total strain of the composite system for different interface elastic modulus. The results are given in Table 3. With the external loading of 80 MPa, when the interface modulus is not very small (greater than 1 GPa), the effect of the interface modulus on the tensile property of the composite material is small. With a 100-fold change of the modulus, from 1 to 100 GPa, the strain changes by about 15%. When the modulus is reduced to 0.001 GPa from 1 GPa, however, the strain increases 50 times. When the loading is 120 MPa and the modulus of the interface is above 0.1 GPa, the strain changes within 10%. When the modulus is reduced to 0.001 GPa, the strain changes by about six times.

Summarising the above calculation results, the elastic modulus of the interface layer influences the stress distribution in the composite material and its total strain. When the interface elastic modulus is greater than the reinforcement elastic modulus, the interface layer will attract the largest stress concentration. On the other hand, when the interface elastic modulus is lower than the matrix elastic modulus by more than two orders of magnitude, the interface is very easy to elastically deform, leading to very large strains of the composite system.

3.2. Effect of Interface Yield Strength on Composite Properties

We have already seen that too large or too small elastic modulus of the interface layer is detrimental to the mechanical performance of the composite system. In this section, when discussing the effect of the interface yield strength, in order to minimise the influence of its elastic modulus, it is fixed at 100 GPa, i.e., mid-way between the modulus values of the matrix and the reinforcing materials. Table 4 gives the maximum stress in the interface layer for different interface yield strength and the externally applied load of 10 and 100 MPa.

From Table 4, when the interface yield strength is increased from 10 to 1000 MPa, the maximum interface stress does not change significantly. If the interface yield strength is low, the stress at the interface is higher than its yield strength, and it will become the weakest region in the composite system. With increasing yield strength of the interface, it cannot take much more stress and so cannot effectively relieve the stress concentration inside the material. Therefore, when the external load is not very large, increasing interface yield strength does not change significantly the internal stress distribution.

For a high interface yield strength fixed at 1000 GPa, to ensure no yielding of the interface, the calculated maximum stress of the interface for different loading of 10, 100 and 500 MPa is 11.9, 119 and 775, respectively, the first two results already included in Table 4. Under such conditions with no interface yielding due to the fixed high interface yield strength, with increasing external load, the maximum interface stress increases as well and remain larger than the external stress.

In summary of the calculations in this section, the interface stress concentration is quite stable and is always larger than the externally applied load. The change of the interface yield strength does not change significantly its stress level. Therefore, it can be concluded that as long as the interface yield strength is slightly larger than the externally applied load, the interface layer can effectively withstand the stress concentration in the entire material.

4. STRESS ANALYSIS USING A MULTILAYER TRANSITION INTERFACE MODEL

The discussion in the last section is all based on the unit cell model containing one interface layer. The conclusion is that both elastic modulus and yield strength of the interface layer do affect the overall composite properties. This proves the earlier discussion about the composite properties being enhanced by good connection between the matrix and reinforcing bodies at their interface.

In reality, the interface between the reinforcing body and the matrix should not be one layer as used in the last section. After the interdiffusion and interaction between the reinforcing body and the matrix, the interface properties more likely change gradually. If there is good interface bonding between the reinforcement and the matrix, such inter-penetration can be more thorough, forming a thicker transition region with a more gradual change of properties in the transition region. Conversely, if there is bad interface bonding between the reinforcement and the matrix, such inter-penetration should be limited, forming a thin transition region, and the property transition would not be as gradual. Under external stress, those interfaces that have large lattice mismatch and where stress concentration is not easily released will become weak regions in the material. Experimental evidence shows that the interface with ceramic reinforcement is usually where fracture starts. In this section, we will use the multilayer interface model to simulate the maximum stress region in the unit cell model [13]. As discussed before, this is along the short axis of the particle. We will apply a stress perpendicular to this short axis.

In order to concentrate our investigation on the effect of interface layers on the composite properties, the following assumptions are made, considering that the yield strength of the reinforcing material is far greater than the matrix material. The reinforcement material is regarded as very rigid, and it does not participate in deformation. The interface layer closest to the reinforcement (left-most layer) has the material parameters of the reinforcement. Such parameters decrease, in an evenly stepped fashion, from the layer closest to the reinforcement to the layer closest to the matrix. The right-most layer is the matrix material. The materials parameters of the different interface layers are shown in Table 5.

4.1. Stress Analysis with Single Interface Layer Model

The model adopting one interface layer means that there is no inter-penetration between the reinforcing body and the matrix. The two just contact each other. Applying different stresses, the resulting stress distribution is shown in Fig. 4.

From Fig. 4, when the externally applied stress is 100 MPa, because the interface layer undertakes some stress concentration, the majority part of the matrix does not yield. The interface layer and the matrix both have elastic deformation, and the maximum stress occurs at the junction between the matrix and the interface, near the loading position (i.e., the top of the modelled area). With increasing external load, after much of the matrix yields, the elastic deformation of the interface layer reduces, and the stress concentration region enlarges. The maximum stress can be more than three times of the loading stress. The part of the matrix near the interface layer has the lowest stress within the entire matrix. Only when the loading reaches 500 MPa does most of the matrix yield. Noting that the matrix yield strength is only 94 MPa, we can see that the high modulus and high strength interface layer shares the majority of the load bearing. Conversely, if the reinforcement strength is low, it is possible to yield far before the average external load reaches its yield strength.

4.2. Stress Analysis with Three Transition Layers

If we increase the number of transition layers from one to three, with elastic modulus 158, 120 and 80 GPa, respectively, and yield strength 1800, 1200 and 600 MPa, respectively, the internal stress distribution under different applied stresses are obtained as shown in Fig. 5.

From Fig. 5, with lower than 100 MPa external loading, because the interface layers undertake some stress, the matrix material does not yield, but elastically deform with the interface layers. The maximum stress occurs in two interface layers, and is lower than in the case of single interface layer, by nearly 40%. Therefore, the continuous interface layers do help withstand the external stress and protect the matrix material. With increasing load, the stress concentration first occurs in the interface layer next to the matrix, but the maximum stress is sill much smaller than in the case of single interface layer. At 500 MPa loading, after the interface layer next to the matrix yields, the maximum stress location moves to the second interface layer. Therefore, the interface layers take the stress concentration in turns, effectively as a safeguard of the composite system.

4.3. Stress Analysis with Six Transition Layers

The complexity of the interface increases with the number of transition layers used. We now increase this to six, with elastic modulus 158, 140, 120, 100, 80 and 60 GPa, respectively, and yield strength 1800, 1500, 1200, 900, 600 and 300 MPa, respectively. Applying different external loading stresses, the internal stress distribution obtained is shown in Fig. 6. It can be seen from this figure that when the applied load is 100 MPa, because the interface layers support some stress, the matrix material does not yield, but instead elastically deform with the interface layers. The maximum stress appears uniformly in the matrix and all the interface layers, achieving a more homogeneous distribution of stress. The maximum stress further reduces compared to the three-layer interface. With increasing external load to 150 MPa, the stress concentration first happens in the interface layer next to the matrix, but the maximum stress reduces significantly compared to the three-layer interface under the same load. With 300 MPa applied load, after the first interface layer next to the matrix yields, the maximum stress moves to the second interface layer.

From these results, it can be concluded that with increasing interface layers, under the same load, the internal stress spreads out and becomes more homogeneous, and the maximum stress decreases. With multiple interface layers, after the layer next to the matrix yields, the stress concentration moves to the next layer. This proves that the interface with transition layers can withstand larger stress compared to straight interface between matrix and reinforcing material. A good interface with the matrix may be even more important than the property of the reinforcing material itself.

4.4. *The Effect of the Transition Interface on the Elastic Modulus in a Unit Cell Model*

For different conditions of the interface as described above, the elastic modulus of the composite material can be calculated, based on the axisymmetric unit cell model. The calculation gives the results of 57.1, 58.2 and 58.8 GPa, for one, three and six transition layers, respectively. With increasing complexity of the interface transition, i.e., the increase of the number of transition layers, the elastic modulus of the composite material increases marginally, no more than 3%.

A more complex transition state of the interface means more gradual and smooth transition of the elastic modulus and the yield strength from the reinforcing body and the matrix. In an ideal case, the best transition should be continuous, i.e., not stepped as the models used here. From the above calculation results, it can be expected that such an ideal interface would increase the composite modulus even more. However, the interface only occupies a small fraction of the volume of the composite or its model, and its presence should not change fundamentally the elastic modulus of the composite. This is the reason for the relatively small influence as far as the elastic modulus is concerned.

A gradual interface means better compatibility between the reinforcing body and the matrix, with no weakness regions. In such case, the stress concentration region moves in a gradual manner, and will not cause sudden cracking or fracture due to the sudden change of material strength in different regions. If the reinforcement and the matrix do not have such good compatibility, the connection interface will have large and sudden strength change. If there is no transition region at the interface, cracking and failure will happen more easily.

5. CONCLUSIONS

The interface and its properties have significant influence over the yield strength and the elastic modulus of the composite systems. In this paper, we have concentrated on the interface and simulated the tensile process of the unit cell model containing an interface layer. Simulation results of stress distribution show the region having the highest stress levels. Concentrating on this region, a layered interface model is designed to resemble the gradual change of modulus and strength from the reinforcing particle to the matrix. Physically, such change could be due to, for example, elemental diffusion between the particle and the matrix, causing a gradual decrease of the property levels in the direction from the harder particle to the weaker matrix. In comparison, the past unit cell models assumed simple interfaces with zero thickness. If the transition interface model can represent the actual transitional state of the interface, it can be used to evaluate the effect of the interface on the elastic modulus and the stress and strain conditions of the composite.

The paper has examined the effect of the elastic modulus and the yield strength of the interface layers and obtained the stress distribution within a unit cell model containing interface layers. A model with multiple transition interface layers is established, and the effect of the number of layers on the stress distribution in and around the interface is discussed. The main conclusions are as follows.

(1) The elastic modulus of the interface layer affects the internal stress distribution of the composite material and the total strain. When the elastic modulus of the interface is very high, the interface layer will take most of the stress concentration, and thus risks fracture. When the elastic modulus of the interface is very low, the interface layer can deform greatly, causing large overall strain in the composite system. This would also result in easy cracking at the interface between the matrix and the reinforcing body.

(2) The stress concentration at one-layer interface is quite stable, and is always higher than the externally applied load. The variation of the yield strength of the interface does not change significantly its load-bearing capability. For the interface layer, its bonding strength controlling fracture is a much more important factor compared to its yield strength.

(3) For interfaces with transition layers, a more gradual and smooth change of material properties within the layers results in spreading and homogenising of the internal stress. It also reduces the maximum stress existing in the material. After the interface layer next to the matrix yields, the stress concentration moves to the next layer. Thus, an interface with multiple transition layers can effectively increase the load-bearing capacity of the composite material, when compared with single, directly bonded interface.

(4) With more gradual and smooth change of material properties in the transition interface layers, the elastic modulus of the composite material

increases slowly, as calculated using the unit cell model. This increase, however, is small and is no more than 3% of the initial elastic modulus based on a simple interface.

The problem addressed here is largely artificial. We imagine that the particle-matrix interface can be described by a gradual transition in properties, with no evidence that such large or extended variations might exist. The models are then solved using standard FEM. The methodology is thus similar to many prior works on graded materials, here with an artificial graded interface. Many papers have been published on this broad topic over many years, with more recent work providing insight into actual crack formation.

ACKNOWLEDGEMENT

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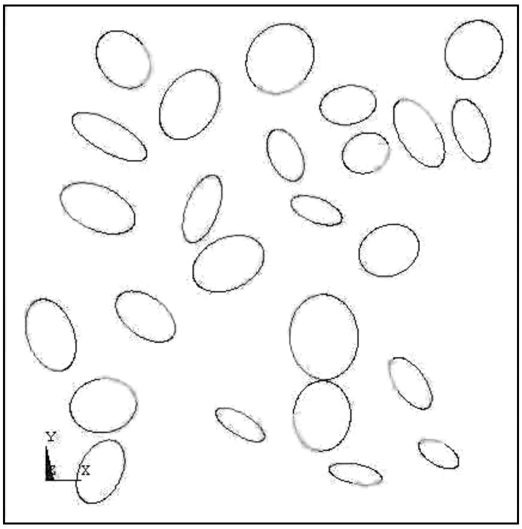

Fig. 1. The model generated randomly distributed spheroidal particles.

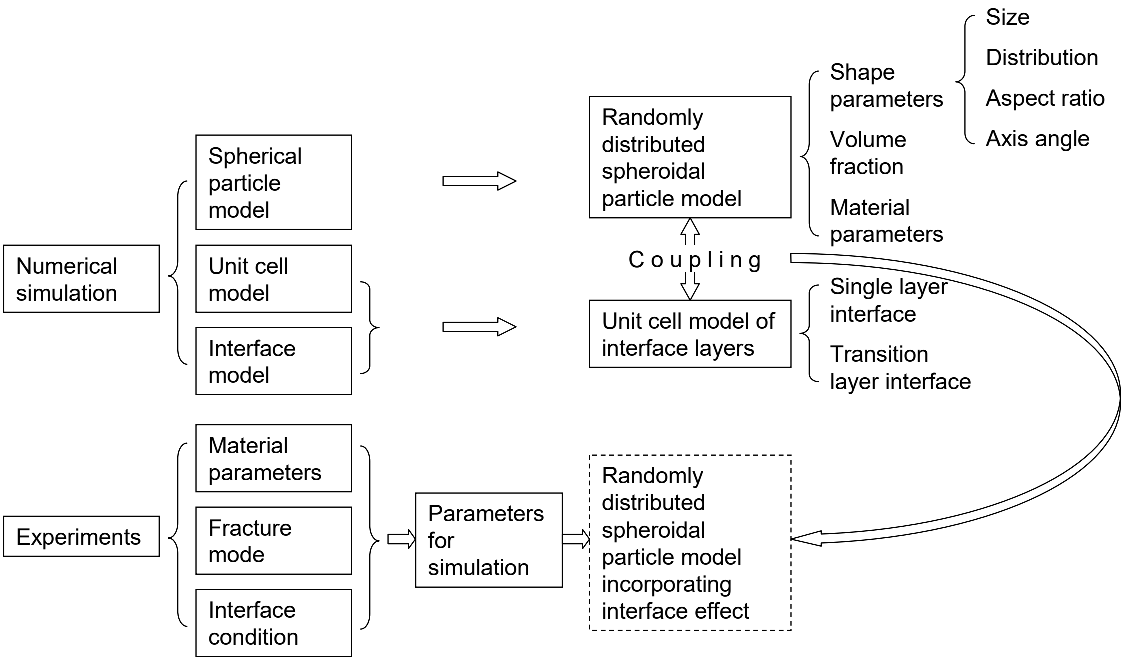

Fig. 2. The coupled model of particle reinforced metal matrix composites.

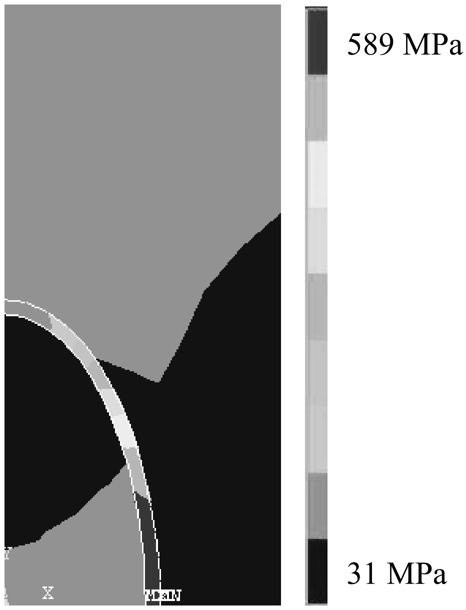

Fig. 3. Stress distribution in the composite for an interface elastic modulus of 1000 GPa and external load of 100 MPa.

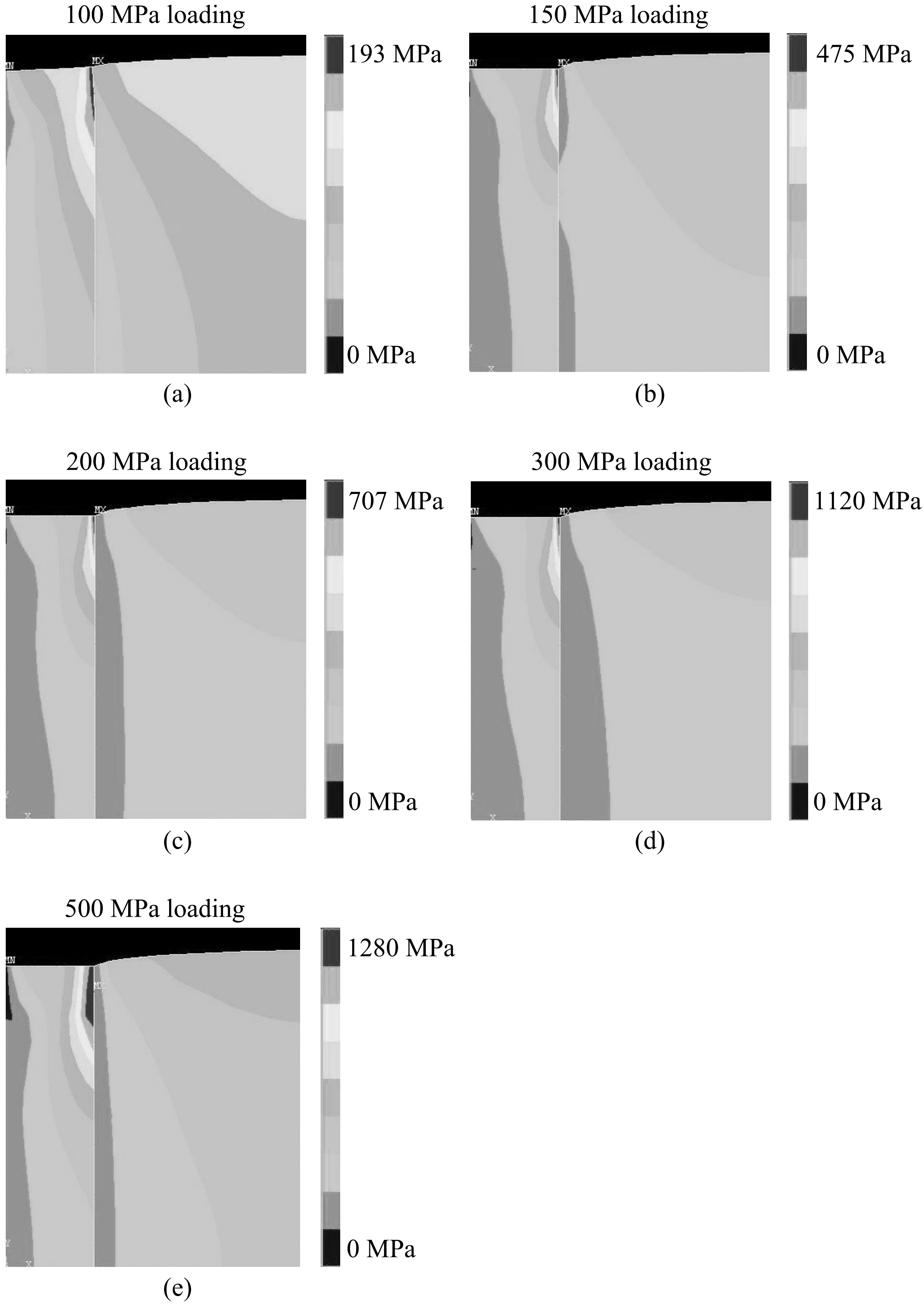

Fig. 4. Stress distribution with single layer interface under different external loading. (a) 100 MPa; (b) 150 MPa; (c) 200 MPa; (d) 300 MPa; (e) 500 MPa.

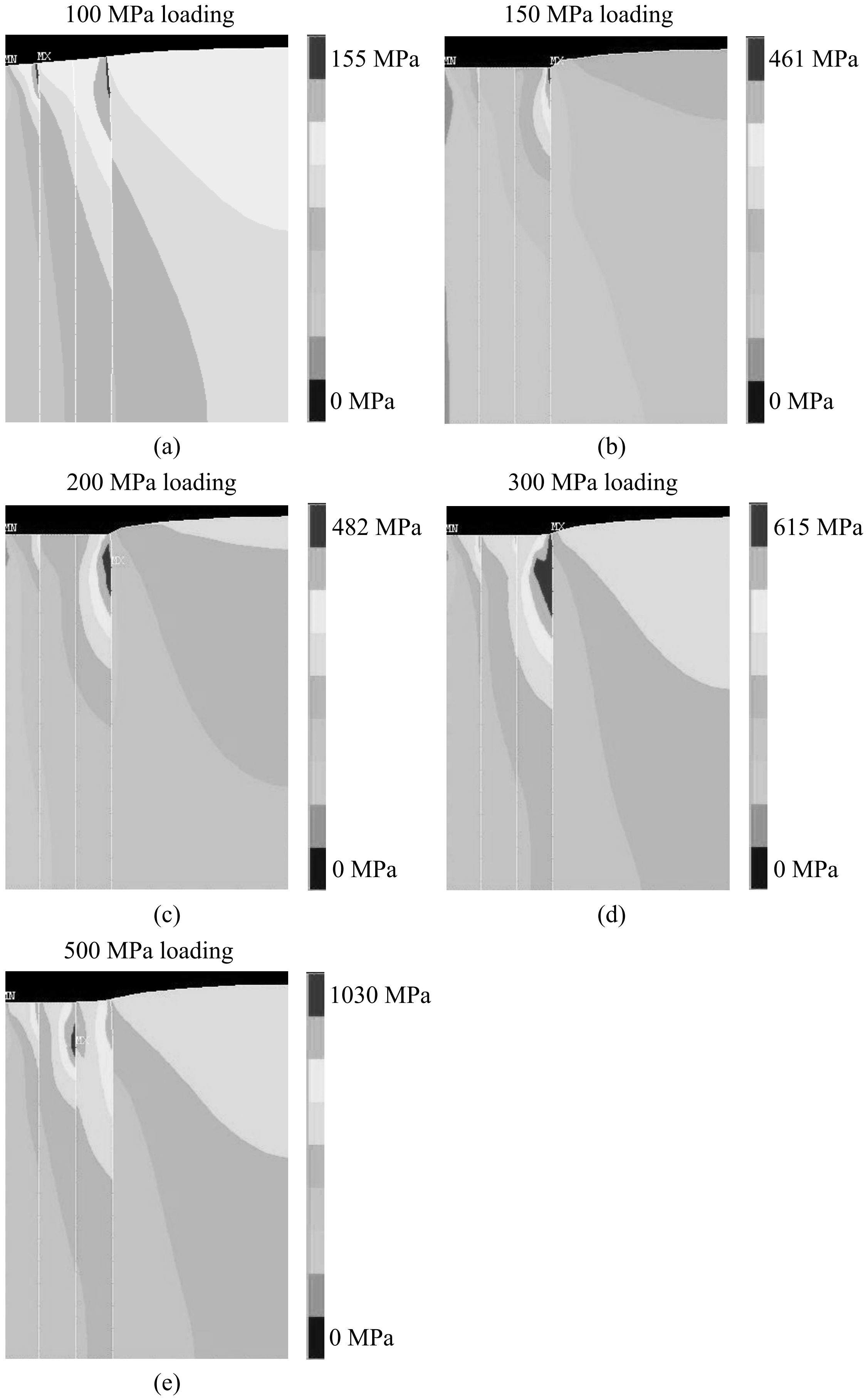

Fig. 5. Stress distribution with three layer interface under different external loading. (a) 100 MPa; (b) 150 MPa; (c) 200 MPa; (d) 300 MPa; (e) 500 MPa.

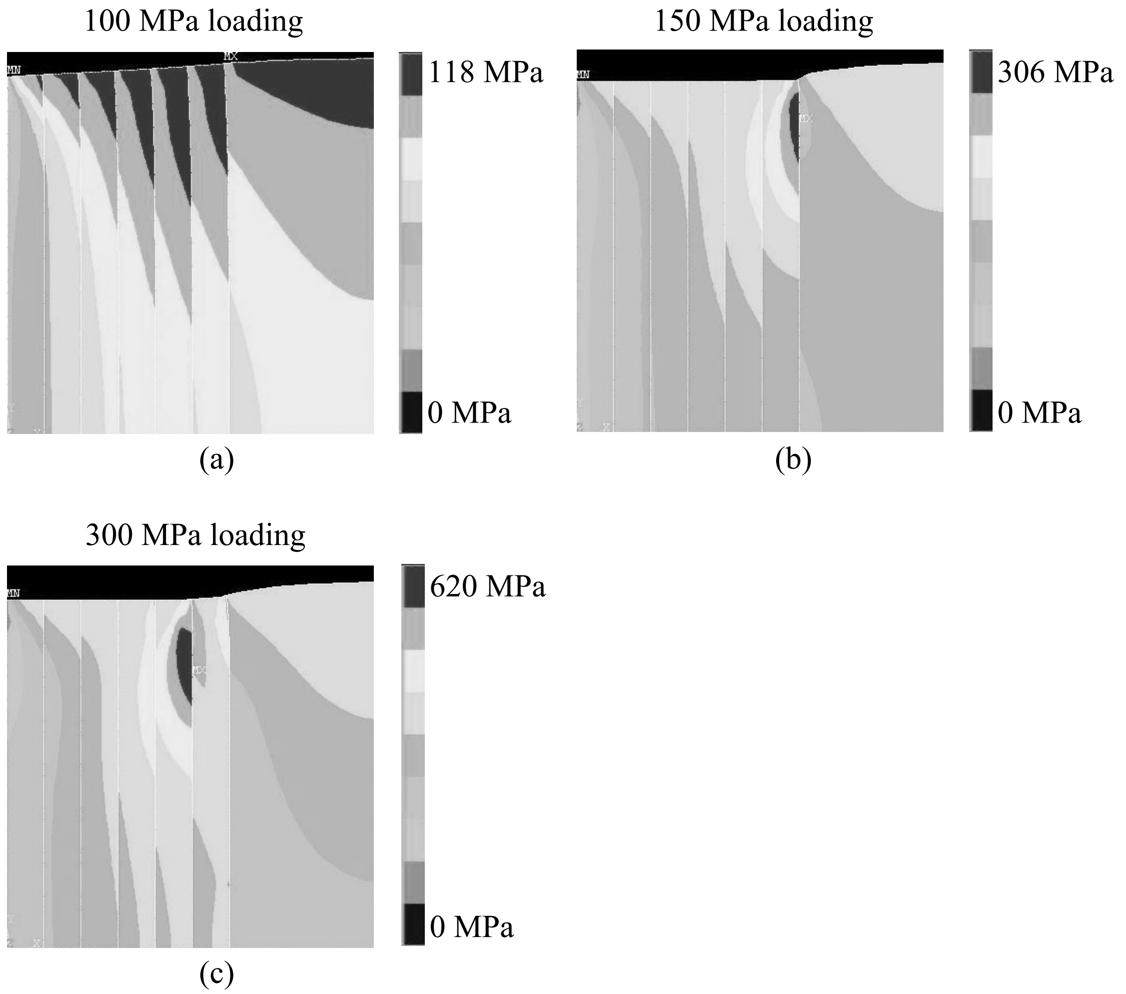

Fig. 6. Stress distribution with six layer complex interface under different external loading. (a) 100 MPa; (b) 150 MPa; (c) 300 MPa.

Table 1. Materials parameters of matrix, reinforcing body and the interface

	Elastic modulus (GPa)	Poisson’s ratio	Yield strength (MPa)	Strain hardening rate (MPa)
Matrix	42	0.33	94	200
Interface	100	0.27	1000	160
Reinforcing body	158	0.205	1800	120

Table 2. Maximum stress in the interface and in the composite system for interface of different elastic modulus and composite under 100 MP loading

Interface elastic modulus (GPa)	Interface maximum stress (MPa)	Composite maximum stress (MPa)
10	116	129
100	119	140
150	137	137
300	238	238
500	360	360
1000	589	589

Table 3. The total strain for different interface modulus and composite under loading of 80 MPa and 120 MPa

Interface elastic modulus (GPa)	80 MPa loading	120 MPa loading
0.001	7.93%	26.2%
0.01	1.61%	10.8%
0.1	0.287%	4.66%
1	0.159%	4.24%
10	0.141%	4.21%
100	0.139%	4.21%

Table 4. Maximum stress in the interface for interface of different yield strength and composite under loading of 10 MPa and 100 MPa

Interface yield strength (MPa)	10 MPa loading	100 MPa loading
10	11.9	100
100	11.9	119
500	11.9	119
1000	11.9	119

Table 5. The elastic modulus and the yield strength of the interface layers.

Number of interface layers	Elastic modulus (GPa)	Yield strength (MPa)
1	158	1800
3	158/120/80	1800/1200/600
6	158/140/120/100/80/60	1800/1500/1200/900/600/300