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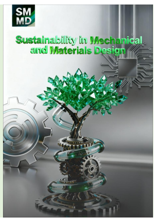

Article

Numerical Simulation Study on the Failure Behavior of Ti-6Al-4V/SiC Composites

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ABSTRACT

The failure behavior of metal matrix composites (MMCs) under extreme environments involves multiple damage mechanisms of the matrix, reinforcement, and interface. Conducting high-fidelity numerical simulations of this behavior remains a significant challenge in the fields of solid mechanics and computational materials science. This paper establishes a numerical simulation framework for Ti-6Al-4V/SiC composites that combines a thermo-mechanically coupled cohesive zone model (CZM) with a ductile phase-field fracture model (PFM). By incorporating the Johnson-Cook (J-C) plasticity and damage criteria, the strain-rate dependent and thermal softening behavior of the titanium alloy matrix is accurately described. Through the development of element and node renumbering strategies, the issue of interrupted phase-field data transfer caused by the embedding of cohesive elements is resolved, enabling effective coupling of interfacial debonding and matrix fracture. The model was validated using smooth round bar tensile experiments; the simulated force-displacement response and damage evolution process show good agreement with experimental results. The results indicate that this model can reasonably predict the entire process of Ti-6Al-4V failure, from damage initiation to macroscopic fracture. This study provides an extensible modeling approach and numerical implementation pathway for the failure analysis of metal matrix composites under complex loading conditions

1. Introduction

Metal matrix composites (MMCs) possess broad application prospects in aerospace, automotive manufacturing, and other fields due to their excellent specific strength, stiffness, and high-temperature performance. Among them, titanium matrix composites, which use titanium alloy as the matrix and ceramics like silicon carbide (SiC) as reinforcements, exhibit good mechanical properties and high-temperature resistance. However, the failure behavior of composites involves multiple

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mechanisms, and accurately predicting their damage evolution process remains challenging. This paper employs a ductile fracture phase-field model (PFM), combined with a thermo-mechanically coupled cohesive zone model (CZM), to conduct numerical simulation and validation of the failure behavior of Ti-6Al-4V/SiC composites.

2. Literature Review

The simulation research on the failure behavior of metal matrix composites (MMCs) has evolved over decades, following a clear trajectory from macroscopic phenomenological models towards multi-scale, multi-mechanism coupled high-fidelity numerical simulations. This development has consistently focused on more realistically capturing the plastic behavior of the matrix, the effects of the reinforcement, and the damage process at the interface.

In the 1980s, the pioneering work of Johnson and Cook laid the cornerstone for the entire field. Their constitutive model proposed in 1983 [1] and the failure criterion established in 1985 [2] systematically described, for the first time, the coupled relationships of strain hardening, strain rate hardening, and thermal softening effects in metallic materials, providing a powerful predictive tool for the response of metals under dynamic loading. Due to its concise form and clear physical significance, this model has been widely adopted and become one of the standard models in impact dynamics.

Building upon the J-C model, numerous scholars have conducted extensive work on calibrating material parameters. Lesuer et al. [3], through systematic experimental studies, provided authoritative J-C plasticity and failure parameters for Ti-6Al-4V, greatly enhancing the simulation accuracy of this alloy in aerospace applications. Concurrently, to better describe the influence of stress state on fracture, Bao and Wierzbicki [4] further revealed the critical role of stress triaxiality on failure strain in their research, correcting the predictive deviation of the J-C failure model under low stress triaxiality and promoting the refinement of failure models.

Entering the 21st century, advancements in computational mechanics gave rise to new paradigms for fracture simulation. The Phase Field Method (PFM) gained favor due to its unique advantages in simulating complex fracture paths (such as branching and merging). The theoretical foundation of this method originates from the variational fracture theory based on energy minimization proposed by Francfort and Marigo [5]. Miehe et al. [6] made landmark contributions on this basis by proposing a thermodynamically consistent fourth-order phase-field fracture model and achieving efficient finite element discretization, establishing a solid computational framework for fracture simulation in both ductile and brittle materials. Subsequently, Borden et al. [7,8] further developed phase-field models suitable for large deformation elasto-plastic problems, successfully coupling the J-C plasticity model with phase-field damage, enabling high-precision simulation of metal ductile fracture.

In recent years, the simulation of multiple failure mechanisms in composites has become a forefront focus. On one hand, researchers are dedicated to developing more refined constitutive models; for instance, the two-scale constitutive model considering non-associated flow proposed by Khan and Liu [9] for Ti-6Al-4V improved predictive capability under complex loading paths. On the other hand, simulating interfacial behavior is crucial. The Cohesive Zone Model (CZM) is widely used to characterize interfacial debonding between reinforcement and matrix, as seen in the classic work of Tvergaard [10]. However, significant technical challenges exist in coupling CZM with PFM to simultaneously simulate matrix fracture and interface failure. A core difficulty is that the insertion of cohesive elements disrupts the topological continuity of the finite element model, leading to failure in phase-field variable data transfer. Scholars like Miehe and Schänzel [11] and Bleyer and Alessi [12] have actively explored this direction, proposing various coupling strategies. It was only recently that studies such as Liu et al. [13] began to systematically address this numerical implementation bottleneck through subroutine development and renumbering algorithms.

In summary, research in this field follows a clear path: "Material Model Innovation" → "Fracture Theory Evolution" → "Multi-physics/Multi-failure Mechanism Coupling". The work presented in this paper is conducted against this backdrop, aiming to solve the numerical implementation challenges associated with the efficient coupling of cohesive zone models and ductile phase-field models, and applying it to titanium matrix composites to achieve more efficient and accurate simulation of their failure behavior.

3. Research Methods

The matrix of metal matrix composites is typically made from alloys such as aluminum, titanium, and magnesium, with reinforcements like SiC, B_4C, and Al_2O_3 added to enhance mechanical properties. This chapter selects titanium alloy as the matrix and SiC as the reinforcement to explore the failure behavior of titanium matrix composites. Firstly, Ti-6Al-4V, as a ductile material sensitive to strain rate and temperature, exhibits a dynamic mechanical response at different temperatures that can be characterized by the Johnson-Cook (J-C) model. Its yield stress σ_y can be written as [2]:

$$\sigma_y = \left(A_{\mathrm{JC}} + B_{\mathrm{JC}}(\bar{\varepsilon}_{\mathrm{p}})^{n_{\mathrm{JC}}}\right)\left[1 + C_{\mathrm{JC}} \ln\left(\frac{\dot{\bar{\varepsilon}}_{\mathrm{p}}}{\dot{\varepsilon}_{\mathrm{ref}}}\right)\right]\left[1 - \left(\frac{T - T_{\mathrm{ref}}}{T_{\mathrm{m}} - T_{\mathrm{ref}}}\right)^{m_{\mathrm{JC}}}\right] \tag{3-1}$$

Where A_{JC} is the initial yield strength of the matrix, B_{JC} and n_{JC} are the strain hardening coefficient and exponent, C_{JC} and m_{JC} are the strain rate and temperature sensitivity coefficients, respectively. The material properties of Ti-6Al-4V are listed in Table 1 [1].

Table 1 Material properties of Ti6Al4V [1]

Elastic Modulus E / GPa	Poisson's Ratio v	Density ρ / kg·m^{-3}	Melting Point T_{m} / K	Specific Heat Capacity c_T / J·(kg·K)$^{-1}$	Thermal Conductivity k_c / W·(m·K)$^{-1}$
109	0.34	4430	1878	611	6.8
A_{JC} / MPa	B_{JC} / MPa	C_{JC}	n_{JC}	m_{JC}	Thermal Expansion Coefficient α_T / K^{-1}
891.5	630.3	0.034	0.547	0.9432	8.8×10^{-6}

Besides the flow stress of the matrix being related to strain rate and temperature, the failure displacement of the matrix is also influenced by these two factors. The widely used Johnson-Cook failure model comprehensively considers factors such as stress triaxiality, strain rate, and temperature. Its specific expression is as follows [2]:

$$\varepsilon_{\mathrm{f}} = \left(D_1 + D_2 \exp\left(D_3 \frac{\sigma_{\mathrm{hyd}}}{\sigma_{\mathrm{eq}}} \right) \right) \left[1 + D_4 \ln\left(\frac{\dot{\bar{\varepsilon}}_{\mathrm{p}}}{\dot{\varepsilon}_{\mathrm{ref}}} \right) \right] \left[1 - D_5 \left(\frac{T - T_{\mathrm{ref}}}{T_{\mathrm{m}} - T_{\mathrm{ref}}} \right) \right] \tag{3-2}$$

Where ε_{f} is the failure strain, σ_{hyd} is the hydrostatic pressure (often related to stress triaxiality η or σ* in the original J-C model); D_1, D_2, D_3, D_4, and D_5 are material parameters, the values of which are listed in Table 2 [14].

Table 2 J-C failure model parameters [14]

Material Parameter	D_1	D_2	D_3	D_4	D_5
Ti6Al4V	0.01546	1.349	−2.144	0.04323	0.6815

Based on literature [4], a damage indicator $D(\bar{\varepsilon}_{\mathrm{p}})$ is introduced to represent damage initiation:

$$D\left(\bar{\varepsilon}_{\mathrm{p}}\right) = \int_0^{\bar{\varepsilon}_{\mathrm{p}}} \frac{d\bar{\varepsilon}_{\mathrm{p}}}{\varepsilon_{\mathrm{f}}(\eta_\sigma, \dot{\bar{\varepsilon}}_{\mathrm{p}}, T)} \tag{3-3}$$

From Eq. (3-3), when $\bar{\varepsilon}_{\mathrm{p}} = \varepsilon_{\mathrm{f}}$, $D(\bar{\varepsilon}_{\mathrm{p}}) = 1$, material damage will occur. Within the ductile fracture phase-field framework, a plastic work threshold is used to control damage initiation instead of the failure displacement, but the two concepts are correlated. Therefore, the plastic work threshold can be further modified as:

$$W_{\mathrm{c}}\left(\eta_\sigma, \dot{\bar{\varepsilon}}_{\mathrm{p}}, T\right) = \bar{\Psi}_{\mathrm{p}} \Big|_{D(\bar{\varepsilon}_{\mathrm{p}})=1} \tag{3-4}$$

Through the treatment in Eq. (3-4), the plastic work threshold can be determined directly from experiments, eliminating the need for repeated adjustments through frequent comparisons between simulation and experiment, which greatly simplifies the process. To verify the reliability of this method, this chapter conducts numerical simulations using the tensile test of a cylindrical bar as an example and compares the results with numerical results from a self-built model in ABAQUS/Explicit and experimental curves [14]. The geometric dimensions and schematic diagram of the tensile test bar are shown in Figure 1.

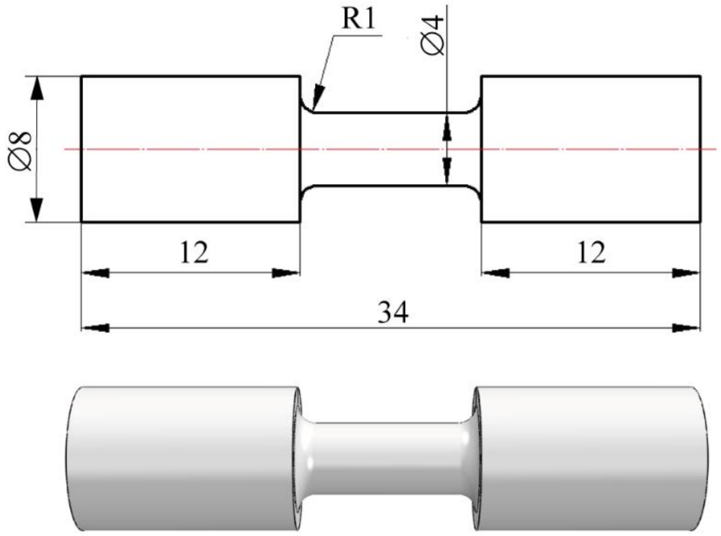

Figure 1 Geometry of the smooth round bar

4. Research Results

A finite element model of the bar was established, and the deformation region was meshed with refinement. The minimum mesh size was 0.2 mm, the element type was C3D8RT (an 8-node linear thermo-mechanical brick element with reduced integration and hourglass control), and the total number of elements was 68,704. Since an explicit solver was used for computation, the time increment was very small. Inputting the actual experimental loading time would result in excessively low computational efficiency. To achieve quasi-static tensile simulation in ABAQUS/Explicit, appropriate mass scaling was applied to the model. According to relevant research [13], when the ratio of kinetic energy to external work/total internal energy during the simulation process is less than 5%, the process can be approximated as quasi-static loading. In this example, the mass scaling factor was chosen as 15. The numerical simulation results are shown in Figure 2.

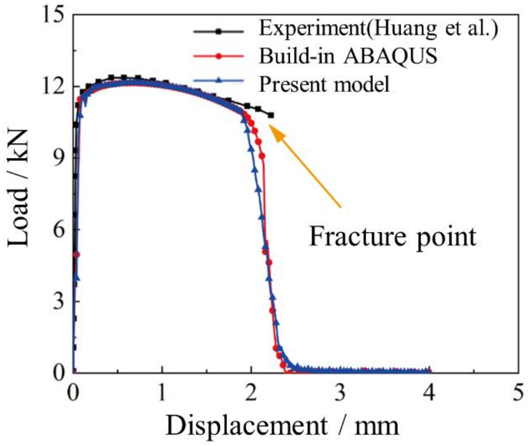

Figure 2 Comparison of force-displacement curves for the smooth round bar

Figure 2 shows the experimental curve, the numerical results from the self-built ABAQUS model, and the numerical results from the current PFM. All three show good agreement. The damage initiation predicted by the self-built ABAQUS model and the current PFM is similar, but certain errors exist. These errors are mainly attributed to the fact that the phase-field model in this chapter does not consider the change in stress triaxiality after damage initiation. In summary, the results indicate that the modified phase-field model can effectively describe the ductile failure behavior of Ti-6Al-4V.

Furthermore, Figure 3 presents the plastic strain and damage evolution process of the smooth cylindrical specimen to further illustrate the model's effectiveness. Figures 3(a) and 3(b) show the equivalent plastic strain (PEEQ) contour plots at damage initiation and when the element is just deleted, respectively. Without considering the effects of strain rate and temperature, the failure strain calculated according to Eq. (3-2) is $\varepsilon_f = 0.6803$, which is close to the result shown in Figure 3(a). Additionally, Figure 3(d) shows the situation at damage initiation . As the load increases, when the phase-field value reaches the critical value for element deletion, i.e., $d \geq 0.9$, elements begin to be removed, as shown in Figure 3(e), and finally, the bar fractures completely in Figure 3(f). These results imply that the current improved ductile phase-field model can effectively predict the mechanical response of Ti-6Al-4V and provides a solid foundation for the next steps of the work.

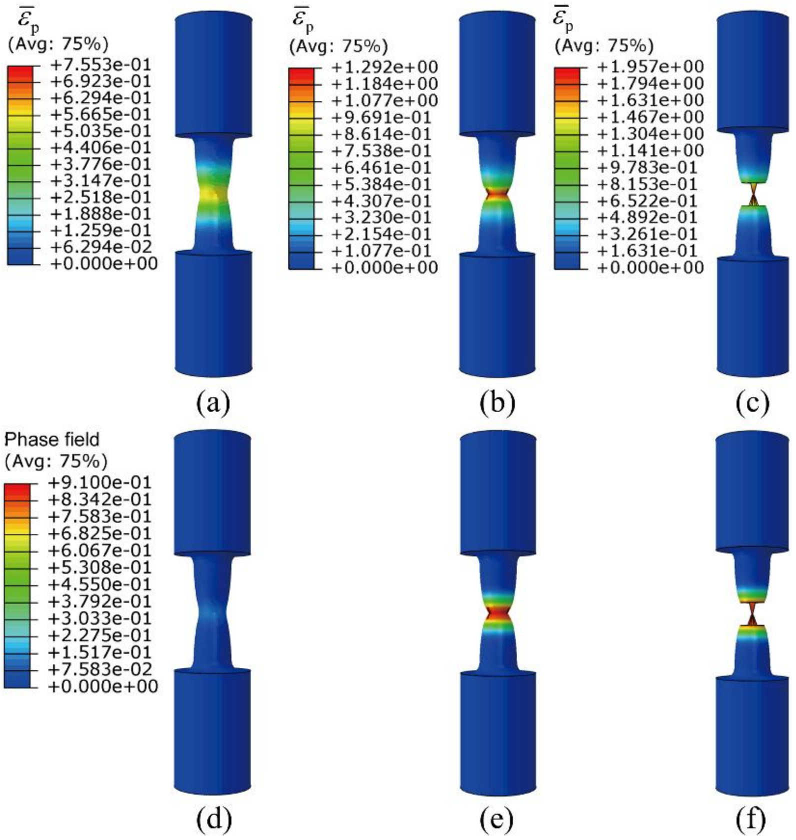

Figure 3 Damage process of the smooth round bar (Elements are deleted when $d \geq 0.9$)

5. Summary and Outlook

This study established a numerical framework integrating a thermo-mechanically coupled cohesive zone model with a ductile fracture phase-field model to simulate the multiple failure behaviors of Ti-6Al-4V/SiC composites. By incorporating the experimentally calibrated Johnson-Cook plasticity and damage models, the mechanical response of the titanium alloy matrix under high strain rates and elevated temperatures was accurately described. To address the key numerical challenges arising from the coupling of the phase-field model and cohesive elements, such as inconsistent element numbering and interrupted data transfer, a solution based on element and node renumbering was proposed. This ensured stable exchange of multi-field variables within the complex model. The results of the smooth round bar tensile simulation demonstrate that the model can effectively predict the damage initiation, evolution, and final fracture process of Ti-6Al-4V material. The numerical results show good agreement with experimental data and those from the built-in ABAQUS model, validating the effectiveness and reliability of the proposed framework.

It is important to emphasize that in the implemented fracture phase-field model, two different parts were used to calculate the displacement field and the phase field separately, but they shared identical element and node numbering, allowing for data exchange via subroutines. The introduction of cohesive elements disrupted the original element and node numbering, causing abnormalities in the data exchange for the fracture phase-field model. Therefore, when combining both for numerical simulation, it is necessary to process the element and node numbering to ensure continuous numbering. Furthermore, within the phase-field model subroutine, the code corresponding to the element and node numbering should be modified so that the element and node numbering of the entire fracture phase-field model maintains a one-to-one correspondence, thereby achieving the combination of the cohesive model and the fracture phase-field model.

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Conflicts of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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