Finite element simulation of real cavity closure in cast Ti6Al4V alloy during hot isostatic pressing

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Abstract: The healing behavior of shrinkage cavity inside the cast Ti6Al4V alloy during hot isostatic pressing (HIP) was investigated experimentally by interrupted hot isostatic pressing tests. The X-ray micro computed tomography was used to record the morphology changes before and after hot isostatic pressing. The two-dimensional geometry obtained by the microCT scan was used in simulation to study the evolution of the real shrinkage cavity during hot isostatic pressing. Shrinkage cavities, shrinkage porosity and small gas pores can be effectively eliminated under proper HIP conditions. The two-dimensional morphology in the simulation results agrees well with the experimental results. This study reveals that plastic deformation, creep and diffusion are the main mechanisms of cavity closure during hot isostatic pressing. In addition, the simplified elliptical pores with aspect ratios at different positions were used to replace the real pores to further study the factors affecting the position of dimples after HIP by simulation. It is found that the position of the dimples mainly depends on the aspect ratio of the elliptical pore and the distance between the pore surface and the external surface of the geometric model.

Keywords: cast Ti6Al4V alloy; hot isostatic pressing; shrinkage cavity; simulation; closure behavior

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1 Introduction

Titanium is an important structural metal and possesses excellent comprehensive mechanical properties ^[1, 2]. In recent decades, Ti6Al4V alloy castings have been widely applied in the aerospace, medical equipment and other industries due to their low density, high specific strength and corrosion resistance ^[3-5]. While Ti6Al4V alloy castings are inherently associated with shrinkage cavities which is ascribed to the poor feeding ability. Hot isostatic pressing (HIP) can eliminate the sealed shrinkage cavities effectively ^[6].

HIP is a process that the high temperature and pressure are imposed to the workpieces to obtain the full-dense components. HIP process has been widely used in castings, and some works have been done on the elimination of the shrinkage cavities in nickel-

based superalloy by HIP process ^[7-10]. However, most of research works focus on the recovery of mechanical property after HIP and few concentrate on the closure process and closure mechanism of shrinkage cavity. And the research on the application of HIP process to Ti6Al4V alloy castings is rarely seen. It is beneficial to optimize the HIP process when the closure behavior of the shrinkage cavity is revealed. Therefore, it is of great importance to study the closure behavior of shrinkage cavity during HIP.

X-ray micro computed tomography (X-ray microCT) is a well-known technique which can quantitatively characterize the morphology of the shrinkage cavity before and after HIP. Du Plessis et al. ^[11-13] has done a lot of work on the quantitative analysis of pores in the as-cast and 3D printed samples before and after HIP using microCT to reveal the details of pore closure. While X-ray microCT is expensive and the pore closure process cannot be recorded in real time. Numerical simulation is much faster and cheaper than the HIP experiments and X-ray microCT tests. And numerical simulation can also visualize the pore closure process during HIP. So, numerical simulation provides an alternative approach to explore the process of pore closure during HIP. Epishin et al. ^[14] studied

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the pore annihilation in a single-crystal nickel-based superalloy by experiment and simulation, and found plastic deformation and diffusion were the two mechanisms for pore closure. Prasad et al.^[15] studied the effect of HIP on the evolution of gas pores using a crystal plasticity finite element model and the model was verified through the comparison with experimental results. The existing studies mainly focus on HIP treatments of nickel-based superalloys, and there are few studies on the evolution process of real pores under the HIP of Ti6Al4V. Studying the evolution of real pores in castings can optimize the HIP process and lay a foundation for the study of pore healing mechanisms. Therefore, research on pore closure in the HIP process of Ti6Al4V alloy by numerical simulation is necessary.

The aim of this study is to explore the kinetics of pore closure and to reveal the pore closure mechanisms during HIP. The method of combining experiment and numerical simulation was adopted to study the evolution of pore closure in the cast Ti6Al4V alloy during HIP. To this end, interrupted HIP experiments and X-ray microCT tests were performed and the simulations of HIP were carried out simultaneously.

2 Material and methods

2.1 Raw material and experimental method

The material used in this study is an investment cast Ti6Al4V alloy, and the chemical composition of Ti6Al4V is listed in Table 1. The casting process was performed in a vacuum induction suspension melting furnace (JISM-20KG/Ti). Before pouring, the molten metal was refined in a water-cooled copper crucible for 3 min, and then the crucible was quickly turned 90° to pour the liquid metal into the pouring cup. The casting parameters were as follows: pouring temperature was 1,720 °C, preheated temperature of the graphite mold was 200 °C, vacuum during melting and casting was 3 Pa, centrifuge speed was 60 rpm. After filling, the centrifuge continued to rotate at a constant speed for 30 min until the liquid metal was completely solidified. After the casting cooled to 200 °C, the graphite mold was broken and the Ti6Al4V alloy casting was taken out from the mold. Samples used in this study were cut from the runners of Ti6Al4V alloy castings. X-ray examination was first used to locate the shrinkage cavity and locations of the shrinkage

Table 1: Chemical composition of as-cast Ti6Al4V alloy (wt.%)

Elements	Ti	Al	V	Si	C	O	N	H	Fe
Content	Bal.	6.40	3.98	0.02	0.014	0.17	0.006	0.002	0.06

cavities were marked on the runner, then runners were cut using wire cut electrical discharge machining (WEDM) to obtain HIP samples with shrinkage cavities in the center.

Interrupted HIP experiments were designed to explore the evolution of shrinkage cavity during HIP. The HIP schedules are depicted in Fig. 1. The black lines represent the temperature, and the red lines represent the pressure. The HIP cycle can be divided into three stages: during the Stage 1, the temperature increased at a rate of 8 °C·min⁻¹, while the pressure increased at a rate of 1 MPa·min⁻¹, until the preset temperature and pressure were reached; in the Stage 2, the temperature and pressure remained unchanged; in the Stage 3, the samples were cooled to 300 °C in the furnace, and part of gas was pump back with a pneumatic pump to ensure that the gas pressure in the furnace was around the standard atmospheric pressure at 300 °C.

The samples were then taken out the furnace followed by air cooling (black arrows in Fig. 1 represent the air cooling). The predetermined temperatures/pressures for HIP-1 and HIP-2 were 780 °C/102 MPa and 920 °C/120 MPa, respectively. There was no holding time (Stage 2) for the preset temperature/pressure of HIP-1, and the holding time for HIP-2 was 1,200 s.

To study the evolution of shrinkage cavities during HIP process, X-ray microCT was used for quantitative 3D measurements before and after HIP treatments. X-ray CT scans were performed on Phoenix v|tome|x m, using 200 kV and 200 μA for X-ray generation. X-ray projection images were recorded at 350 ms per image, with 1,600 images in one full rotation, and the voxel size was set to 16 μm.

2.2 Computation method

HIP process is a coupled thermo-mechanical process. Large deformation occurs around the pore in the castings to close the pore during HIP. The total strain can be decomposed into the thermal, elastic and inelastic strains as shown in Eq. (1)^[16, 17]:

$$\varepsilon_{ij} = \varepsilon_{ij}^{th} + \varepsilon_{ij}^{el} + \varepsilon_{ij}^{inel} \quad (1)$$

where ε_{ij} is the total strain, ε_{ij}^{th} is the thermal strain, ε_{ij}^{el} is the elastic strain and ε_{ij}^{inel} is the inelastic strain. The inelastic strain can be decomposed into time independent inelastic strain (plastic strain) and rate dependent inelastic strain (creep strain). The total strain can be expressed as Eq. (2):

$$\varepsilon_{ij} = \varepsilon_{ij}^{th} + \varepsilon_{ij}^{el} + \varepsilon_{ij}^{pl} + \varepsilon_{ij}^{cr} \quad (2)$$

where ε_{ij}^{pl} is the plastic strain and ε_{ij}^{cr} is the creep strain. It's

Fig. 1: Temperature and pressure versus time profile for HIP-1 (dotted line) and HIP-2 (solid line)

well-known that the bilinear elastoplastic model and time-hardening creep model were used to calculate $\Delta\varepsilon_{ij}^{pl}$ and $\Delta\varepsilon_{ij}^{cr}$. The change of thermal strain can be expressed as Eq. (3).

$$\Delta\varepsilon_{ij}^{th} = \alpha(T) \Delta T \delta_{ij} \quad (3)$$

where $\alpha(T)$ is the thermal expansion coefficient which depends

on temperature T , ΔT is the change of temperature during HIP, δ_{ij} is the Kronecker Delta. The temperature-dependent thermal-mechanical parameters used in this study are shown in the Table 2. The density and thermal expansion coefficient are defined as constant, the values are $4.31 \text{ g}\cdot\text{cm}^{-3}$ and $9.9\text{E-}6 \text{ }^\circ\text{C}^{-1}$, respectively.

Table 2: Temperature-dependent thermal and mechanical properties of as-cast Ti6Al4V alloy [5, 18-20]

Thermo-mechanical properties	Temperature ($^\circ\text{C}$)					
	25	200	400	600	800	920
Thermal conductivity ($\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$)	6.70852	8.36265	10.6828	12.6755	15.1622	16.4327
Specific heat ($\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$)	550	569	612	655	698	646
Young's modulus (GPa)	112	104	92	76	56	42
Poisson's ratio	0.34	0.34	0.37	0.39	0.41	0.42
Yield strength (MPa)	887	668	508	390	119	30
Tangent module (MPa)	1,329	1,210	1,054	890	721	617

The numerical simulations were performed using the commercial finite element software ABAQUS. The temperature and pressure loads were applied to the outer surfaces of the model. The input parameters of temperature and pressure could be obtained from Fig. 1. Self-contact was defined on the pore surface to simulate the contact behavior of pore surfaces during HIP. A reference point on the external surface was fixed to ensure that there was no rigid motion during the simulation.

3 Results and discussion

3.1 Closure mechanism of shrinkage cavity during HIP

Figure 2 presents the 3D semi-transparent view with color coding of pores based on their volume before and after HIP. Before HIP, there is one big shrinkage cavity, shrinkage porosity, some small gas pores and some pores connect to the external surface (as indicated by the arrows with different

colors in Fig. 2). The initial porosity is 1.167%. After HIP-1, there is no obvious change in the morphology and volume of the pore, and the porosity is 1.1% [Fig. 2(b)]. After HIP-2, the shrinkage cavity, shrinkage porosity and gas pore are all closed, only the pores connect to the external surface remained, the porosity is 0.0028% [Fig. 2(c)]. It is obvious that HIP can effectively eliminate shrinkage cavities, shrinkage porosity and small gas pores under proper HIP conditions.

The morphology of the shrinkage cavity is complex which has the geometric features of sharp corners and small channels. The simulation is difficult to converge when the real 3D geometry is used in the simulation. Therefore, the 3D problem is simplified to the 2D problem to study the evolution process of the pores in the cross sections during HIP treatment. According to the X-ray microCT scan results after HIP-2, the positions of the dimples are measured [see Fig. 3(a)], and then cross sections are made at the marked positions of the X-ray microCT scan results before HIP [see Fig. 3(b)]. The volume of shrinkage cavity is the largest, so only the shrinkage cavity

Fig. 2: 3D views of sample with color-coded pores according to volume from 3D analysis: (a) before HIP; (b) after HIP-1; (c) after HIP-2

is considered. Other shrinkage porosity and gas pores are ignored to simplify the study. The geometry of Section A and Section B with the finite element mesh are shown in Figs. 3(c) and (d), respectively. In addition, pore closure occurs according to two main steps in the hot forging^[21]: mechanical closure and diffusion bonding. The mechanical closure leads to the contact

between the internal pore surfaces, and the diffusion bonding leads to the bonding of contact surfaces and a full-dense alloy is finally obtained. HIP is similar to the hot forging process. Therefore, there are also two steps in the process of pore closure during HIP. Only the mechanical closure of the cavity was considered in the simulation.

Fig. 3: Location of dimple after HIP-2 (a), location of sections before HIP (b), finite element mesh of Section A and Section B (c, d). Red arrows indicate locations and directions of paths mentioned in Fig. 8

Figure 4 shows the distribution of the equivalent plastic strain (PEEQ) and equivalent creep strain (CEEQ) in Section A and Section B during HIP-1. Plastic deformation occurs at $t=5,290$ s in Section A, while the plastic deformation occurs at $t=5,601$ s in Section B. The stress concentration at the corner of Section A causes the plastic deformation to start early. Generally speaking, creep is usually considered to occur when temperature exceeds $0.3T_m$ ^[22] (T_m is the melting temperature, the melting temperature of Ti6Al4V alloy is $1,655$ °C; $0.3T_m$ is about 500 °C). HIP temperature is 500 °C at $t=3,750$ s. Creep strain can occur when the equivalent stress is less than the yield stress, while only when the equivalent stress is greater than or equal to the yield stress, the material will

undergo plastic deformation. Therefore, creep starts earlier than plastic deformation. The plastic strain is time-independent and creep strain is rate-dependent, which means that the plastic strain does not accumulate over time while the creep strain accumulates continuously in the fixed boundary condition. Therefore, creep lasts longer than plastic deformation. To summarize, due to the longer time and larger strain rate of creep^[23], it is reasonable that the creep strain is larger than the plastic strain. After HIP-1, there are no obvious geometry changes in Section A and Section B. The maximum values of PEEQ and CEEQ in Section A and Section B are all located around the shrinkage cavity after HIP-1.

Fig. 4: Distribution of PEEQ and CEEQ during HIP-1: (a) Section A; (b) Section B

Figures 5 and 6 show the distribution of PEEQ and CEEQ in the Section A and Section B during HIP-2, respectively. In Section A, the size of the cavity in the Y direction is approximately half of the size in the X direction. Thus, the final healing interface is perpendicular to the Y direction (see Fig. 5). The cavity is approximately located at the center, and

a dimple is formed on the top surface perpendicular to the closing direction of the cavity. Similarly, the shrinkage cavity in the Section B has a larger size in the Z direction than in the Y direction, therefore the healing interface is perpendicular to the Y direction and a dimple is formed on the right surface (see Fig. 6). In addition, the dimple is also formed on the upper

Fig. 5: Distribution of PEEQ (a) and CEEQ (b) in Section A during HIP-2

Fig. 6: Distribution of PEEQ (a) and CEEQ (b) in Section B during HIP-2

surface which could be ascribed to that the pore surface is closer to the top surface than the right surface. After HIP-2, the cavities on the different sections are all closed, and some dimples are formed on the external surfaces. The maximum plastic strain and creep strain are on both sides of the healing interface after HIP-2. The morphologies of Section A and Section B after HIP-1 and HIP-2 experiments are shown in Fig. 7. The simulation results agree well with the experimental results.

After HIP-2, the PEEQ and CEEQ along Paths defined in Fig. 3(c-d) are presented in Fig. 8. The dimples are formed along Path 3, Path 6 and Path 7, which indicate that the cavity is closed mainly along Path 3 in Section A and Path 6 and Path 7 in Section B. It can be seen the plastic strain and creep strain mainly located around the cavity and the dimple. The creep strain is larger than the plastic strain during HIP treatment of Ti6Al4V alloy, which is ascribed to the long time and high strain rate^[23] of the creep deformation under high temperature and high pressure.

The above simulation results indicate that the cavity is closed mainly by plastic deformation and creep. Atkinson et al.^[24] found that as higher densities were approached during the HIP treatment of powder, pores were filled by diffusion. Similarity, the touched interfaces

after the mechanical closure need to be bonded through diffusion to be fully closed^[21]. Therefore, the main mechanisms of the cavity closure during HIP treatment of Ti6Al4V alloy are plastic deformation, creep and diffusion.

Fig. 7: Experimental results after HIP-1: (a) Section A and (b) Section B; after HIP-2: (c) Section A and (d) Section B

Fig. 8: Distribution of PEEQ (a) and CEEQ (b) along Paths 1–4 [Fig. 3(c)] in Section A after HIP-2, and distribution of PEEQ (c) and CEEQ (d) along Paths 5–8 [Fig. 3(d)] in Section B after HIP-2

3.2 Position of dimple after HIP

To further explore the positions of dimples after HIP, numerical simulations were carried out to study the shape change of geometric model with elliptical pores inside (see Fig. 9). The geometry and dimensions of elliptical pores are shown in Figs. 9(a) and (b). The aspect ratios of ellipses are

1:1, 7:6, 7:5, 7:4, 7:3, 7:2 and 7:1, numbered 0 to 6 in order. The aspect ratio of the No. 0 ellipse is 1, which means that the No. 0 ellipse is a circle with a radius of r . Ellipses whose major axes are parallel to the Y -axis are marked as I [see Fig. 9(a)], and ellipses whose major axes are parallel to the X -axis are marked as II [see Fig. 9(b)].

Fig. 9: Geometry and dimension of elliptical pores: (a) major axis of elliptical pores along Y -axis; (b) major axis of elliptical pores along X -axis; (c–e) geometric models for numerical simulations of HIP

The center of elliptical pore is located at three different positions inside geometric model, these three cases are marked as Case 1, Case 2 and Case 3, as shown in Fig. 9(c–e). In Case 1, the center of the ellipse is on the diagonal of the geometric model [see Fig. 9(c)]. Due to the symmetry, the elliptical pores whose long axes are parallel to the Y -axis are only considered. In Case 2, the center of the ellipse moves along the Y -axis direction, and the position of the ellipse along the X -axis direction remains unchanged, causing the center of the ellipse to be closer to the upper surface [see Fig. 9(d)]. Two types of elliptical pores, I and II, are considered. In Case 3, the center of the elliptical pore moves along the X -axis direction, while the position of the elliptical pore along the Y -axis direction remains unchanged [see Fig. 9(e)]. Compared to Case 2, elliptical pores are farther from the left surface. Similarly, two types of elliptical pores, I and II, are considered. The relative positions of the center of elliptical pores (A, B and C) in three

cases are illustrated in Fig. 9(e). The minimum distances between the surface of the elliptical pore and the surface of the geometric model in two mutually perpendicular directions are marked as a and b , respectively, where $a \geq b$. a and b in Fig. 9(c–e) refer to the shortest distance between the surface of the elliptical pore numbered 6 of type I and the surface of the geometric model. All discussions and conclusions are based on the assumption that a is less than or equal to $\frac{7r}{2}$ and b is greater than or equal to $\frac{r}{2}$ to ensure that the center of the elliptical pore is not too far or too close to the surface of the geometric model.

After HIP simulations, the positions of dimples are summarized in Table 2. It can be found that in the three cases, dimples are all formed on the surface closest to the pores when the aspect ratio of the elliptical pore is 1 (the elliptical pores numbered 0).

Table 2: Positions of dimples after HIP simulation

Case		Number of elliptical pore						
		0	1	2	3	4	5	6
1	I	Left and Top	Left	Left	Left	Left	Left	Left
	II	Top	Top	Left and Top	Left	Left	Left	Left
2	I				Top			
	II							
3	I				Top			
	II							

In Case 1, it can be found that the distance between the pore surface and the left surface of geometric model is greater than or equal to the distance between the pore surface and the top surface of geometric model. For the elliptical pores numbered 1–6, dimples are all formed on the left surface of geometric models after HIP simulations, indicating that when $1 < a:b \leq \frac{13}{7}$ (the elliptical pores numbered 1–6), the position of the dimple is only related to the direction of the minor axis of the ellipse, that is, the dimple appears on the surface perpendicular to the minor axis of the ellipse.

In Case 2, when the major axis of the ellipse is parallel to Y -axis, dimples appear on the left side in most situations, indicating that when $\frac{18}{7} \leq a:b \leq \frac{26}{7}$ (the elliptical pores numbered 2–6), the position of the dimple is related to the direction of the minor axis of the ellipse, that is, the dimple appears on the surface perpendicular to the minor axis of the ellipse. Only when the aspect ratio of the ellipse is less than or equal to $\frac{7}{5}$ ($2 \leq a:b \leq \frac{18}{7}$, the elliptical pores numbered 0–2), dimples are generated on the top surface, which shows that the position of the dimple is affected by the distance between the pore surface and the external surface of geometric model and the aspect ratio of the elliptical pore. When the major axis of the elliptical pore is parallel to the X -axis, the dimples all

appear on the top surface, indicating that when $\frac{15}{14} \leq a:b \leq \frac{14}{9}$, the dimple appears on the surface perpendicular to the minor axis of the ellipse.

In Case 3, when the major axis of the ellipse is parallel to Y -axis, dimples all appear on the top surface, the position of the dimple only relates to the shortest distance from the pore surface to the surface of the geometric model, that is, when $a:b \geq 5$ (the elliptical pores numbered 0–6), the dimple appears on the surface of the geometric model closest to the pore surface. When the major axis of the elliptical pore is parallel to the X -axis, the dimples all appear on the top surface, indicating that when the ellipse is closest to a certain surface of the geometric model along the minor axis, dimples will definitely appear on this surface.

To summarize, the formation position of the dimple is related to the aspect ratio of the ellipse and the distance between the pore surface and the outer surface of the geometric model. The following laws are summarized: (1) when the aspect ratio of the elliptical pore is 1, a dimple forms on the surface closest to the pore surface; (2) when $1 < a:b \leq \frac{13}{7}$ and $\frac{18}{7} \leq a:b \leq \frac{26}{7}$ are satisfied, a dimple appears on the surface perpendicular to the minor axis of the ellipse; (3) when $a:b \geq 5$, a dimple appears on the surface closest to the pore surface; (4) when the ellipse is closest to a certain surface of the geometric model along

the minor axis, dimples will definitely appear on this surface.

For the pore in Section A (Section 3.1), $a:b = \frac{11}{8}$, the dimple appears on the surface perpendicular to the minor axis of the ellipse, which agrees with (2). For the pore in Section B, $a:b = \frac{17}{7}$ and the aspect ratio is equal to $\frac{7}{5}$, the ellipse is similar to the elliptical pore numbered 2 of type I in Case 2, the dimples appear on the surface closest to the pore surface and the surface perpendicular to the minor axis, which agrees with the result of the elliptical pore numbered 2 of type I in Case 2.

4 Conclusions

The healing behavior of the shrinkage cavity in the cast Ti6Al4V alloy was studied by experiments and simulation. The relationship between the position of dimples and the aspect ratio of the elliptical pore, and the distance between the pore surface and the outer surface of the geometric model was also explored by simulation. The main conclusions can be summarized as follows:

(1) Proper HIP can effectively eliminate the centimeter-scale shrinkage cavity, shrinkage porosity and small gas pores.

(2) The healing behavior of the shrinkage cavity inside the cast Ti6Al4V alloy could be modelled by the plasticity and creep models. The simulation results agree well with the experimental results.

(3) The main mechanisms of cavity closure during HIP of the cast Ti6Al4V alloy are plastic deformation, creep and diffusion.

(4) The formation position of dimples is related to the aspect ratio and location of the elliptical pores.

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