Using morphology-equivalent method to simulate the evolution of shrinkage in Ti6Al4V alloy castings during HIP

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Abstract. Hot isostatic pressing (HIP) is an effective method to eliminate the shrinkage in castings. The morphology of shrinkage is complex, and there are structures such as sharp corners and small passages which would lead to a large number of elements and easily divergent calculation results. Therefore, the application of numerical simulation in HIP is limited. To solve the non-convergence problem, the real shrinkage is often simplified as a sphere. However, this simplification ignores the characteristics of the shrinkage and makes the simulation results unreliable. In this paper, the technique of morphology-equivalent ellipsoid is applied to the numerical simulation of shrinkage evolution during HIP. Firstly, the 3D morphology of shrinkage in Ti6Al4V alloy castings is obtained by micro computed tomography. The radius of sphere and the geometric size and orientation of morphology-equivalent ellipsoid are calculated by corresponding equivalent techniques. Secondly, the numerical simulations of HIP for the Ti6Al4V castings before and after the equivalent method are carried out. The volume evolution of three kinds of shrinkages are recorded and compared. The results show that the volume evolution of the morphology-equivalent ellipsoid is closer to that of the real shrinkage, the feasibility of the morphology-equivalent ellipsoid and the limitations of sphere are verified.

1. Introduction
Ti6Al4V alloy is widely used in the aerospace industry due to their low density, high specific and corrosion resistance. During the casting of Ti6Al4V alloy, the metal liquid is difficult to feed as a result of poor fluidity, and the defect such as shrinkage is easily generated. Hot isostatic pressing (HIP) is a well-known method to eliminate the shrinkage in castings and improve material properties[1].

HIP is a process that the castings or powder is densified under the action of high temperature and high pressure. The current research on HIP of castings is mainly based on experimental methods. Anton du Plessis et al. [1] firstly applied x-ray microcomputed tomography (Micro-CT) to quantify the shrinkage changes before and after HIP of as-cast Ti6Al4V rods. Chung-Hung Tam et al. [2] have studied the effects of the HIP temperature on Cr-Si targets and found suitable HIP temperatures. X.G. Zheng et al. [3] explored the healing process of shrinkage in a Ni-based superalloy by HIP. Numerical simulation is another effective way to study the process of shrinkage elimination during HIP due to their low cost and predictive ability. However, there are few researches on numerical simulation of HIP. Alexander Epishin et al. [4] gave the kinetics of pore annihilation during HIP by experiment and modelling. Yu Zhou et al. [5] proposed a healing model for creep cavities under HIP. In our previous research [6], the effects of temperature on the shrinkage densification and microstructure of Ti6Al4V alloy have been...
studied by experimental and numerical simulation methods. In all existing numerical simulations of HIP, it is assumed that the shrinkages in the castings are spherical, ignoring the morphology of the real shrinkage. That is because the real shrinkage morphology often has complex geometric features such as sharp corners and small passages which will lead to the diverging simulation results. Therefore, it is meaningful to solve the non-convergence problem during HIP.

In previous studies, an equivalent method using ellipse or ellipsoid to replace the real shrinkage was employed in forging process. Kieran F. Mulchrone et al.[7] fitted an ellipse to an arbitrarily shaped region for strain analysis. M. Saby et al.[8] used the morphology-equivalent ellipsoid to analyze the void closure during forge. This paper refers to the equivalent method of shrinkage in forging, and applies this method to the numerical simulation of HIP for Ti6Al4V alloy. The volume evolution of real shrinkage, volume-equivalent sphere and morphology-equivalent ellipsoid are compared and discussed.

2. Equivalent method

The morphology of the castings and shrinkage was obtained from the Micro-CT, as shown in figure 1.

![Figure 1. The morphology of the casting and the shrinkage.](image)

2.1. The volume of the shrinkage

The binary STL files were obtained from the Micro-CT, which contain the information of triangles. The volume of the shrinkage can be expressed as Eq. (1):

\[
\frac{1}{6} \sum_{\tau \in T} \begin{vmatrix}
    x_{\tau,1} - x_0 & y_{\tau,1} - y_0 & z_{\tau,1} - z_0 \\
    x_{\tau,2} - x_0 & y_{\tau,2} - y_0 & z_{\tau,2} - z_0 \\
    x_{\tau,3} - x_0 & y_{\tau,3} - y_0 & z_{\tau,3} - z_0
\end{vmatrix}
\]

(1)

where \( \tau \) is a triangle of the surface mesh \( T \) of the shrinkage, \( x_{\tau,i}, y_{\tau,i} \) and \( z_{\tau,i} \) \((i = 1, 2, 3)\) are the coordinates of the three vertices of triangle \( \tau \), \( x_0, y_0 \) and \( z_0 \) are the coordinates of origin.

Encode Eq. (1) with Python, the volume of the shrinkage is 8.4802mm\(^3\). The equivalent spherical shrinkage has the same volume with the real shrinkage. Therefore, the radius of the equivalent spherical shrinkage is 1.2650mm.

2.2. Generation of the morphology-equivalent ellipsoid

The morphology-equivalent ellipsoid is generated in order to represent shape factors and principal orientations of real shrinkage accurately[8]. The schematic diagram of the construction process of the morphology-equivalent ellipsoid is shown in the figure 2. First, the shape factors and principal orientations of inertia ellipsoid are obtained by computing the inertia matrix of the real shrinkage. Then, the morphology-equivalent ellipsoid is obtained by volume correction of the inertia ellipsoid. And the inertia matrix can be represented as:

\[
\begin{bmatrix}
    I_{xx} & -I_{xy} & -I_{xz} \\
    -I_{xy} & I_{yy} & -I_{yz} \\
    -I_{xz} & -I_{yz} & I_{zz}
\end{bmatrix}
\]

(2)
where $I_{xx}$, $I_{yy}$ and $I_{zz}$ are the moment of inertia of the rigid body relative to the coordinate axis, $I_{xy}$, $I_{xz}$, $I_{yx}$, $I_{zx}$ and $I_{zy}$ are the inertia product of the rigid body relative to the coordinate axis, and they are defined as:

\[
\begin{align*}
I_{xx} &= \iiint_G \left( y^2 + z^2 \right) dx
dy
dz \\
I_{yy} &= \iiint_G \left( x^2 + z^2 \right) dx
dy
dz \\
I_{zz} &= \iiint_G \left( x^2 + y^2 \right) dx
dy
dz \\
I_{xy} &= \iiint_G xy
dx
dy
dz \\
I_{xz} &= \iiint_G yz
dx
dy
dz \\
I_{yx} &= \iiint_G yx
dx
dy
dz \\
I_{zx} &= \iiint_G zx
dx
dy
dz \\
I_{zy} &= \iiint_G zy
dx
dy
dz
\end{align*}
\]

Figure 2. Schematic diagram of the process for calculating the morphology-equivalent ellipsoid.

The matrix shown by Eq. (2) is a symmetric matrix whose eigenvalues are the lengths of three semi-axes of the inertia ellipsoid, and the eigenvectors are the principal axes of the inertia ellipsoid. The length ratio and the principal orientations of the three semi-axes of the inertia ellipsoid are kept unchanged, and the semi-axes of the inertia ellipsoid is scaled so that the transformed volume is equal to the volume of the real shrinkage. The ellipsoid obtained by the inertia ellipsoid transformation is the morphology-equivalent ellipsoid. The morphology-equivalent ellipsoid is shown in figure 3 with red color superimposed with the real shrinkage in green color and volume-equivalent sphere in blue color.

Figure 3. The real shrinkage, morphology-equivalent ellipsoid and volume-equivalent sphere.

Figure 4. Boundary conditions and variation of pressure and temperature with time in a HIP cycle.
3. FEM simulation
The numerical simulations of HIP process for the Ti6Al4V alloy castings with three kinds of shrinkage were carried out using the finite element software ABAQUS. The fixed boundary was applied to the bottom surface of the geometry, a temperature boundary and a pressure load were applied to each face of the geometry, as shown in figure 4(a). The curves of temperature boundary and pressure load versus time are shown in figure 4(b). During the HIP process, the temperature and pressure simultaneously increased to 930 °C and 120 MPa, and maintained for 50min, and then decreased to 25 °C and 1E-5 MPa, respectively.

4. Simulation results and discussion
The morphology evolution of real shrinkage, morphology-equivalent ellipsoid and volume-equivalent sphere are shown in figure 5(a). The closure process of the casting with real shrinkage cannot reach the end of simulation due to the mesh distortion. While it still can be found that the morphology-equivalent ellipsoid has the same closure tendency as the real shrinkage hole, that is, the change of shrinkage is small in the long axis direction, and the shrinkage closure is mainly dependent on the collapse in the short axis direction. However, the volume-equivalent sphere exhibits equal shrinkage in almost all directions.

![Figure 5](image)

**Figure 5.** The FEM analysis of the morphology change and the volume evolution of real shrinkage, the morphology-equivalent ellipsoid and volume-equivalent sphere under HIP.

The volume evolution of real shrinkage, the morphology-equivalent ellipsoid and volume-equivalent sphere are plotted in figure 5(b). It can be seen that the volume-equivalent sphere underestimates the real closure degree during HIP which may be ascribed to the tortuosity of the surface of real shrinkage. Some of the initial morphology must be favorable to void closure[8]. The morphology-equivalent ellipsoid underestimates slightly the real closure degree and it agrees well with the real shrinkage. Therefore, using the morphology-equivalent ellipsoid to replace the real shrinkage will have better prediction results. The result also reveals that the flatten-shaped shrinkage[9] can be healed easily.

5. Conclusion
In this study, the morphology-equivalent method was used to simulate the elimination of shrinkage in Ti6Al4V alloy castings during HIP. Important conclusions are presented below.

(1) The morphology of real shrinkage is so complicated that the numerical simulation of HIP for castings is difficult to be carried out. Replacing the real shrinkage with the morphology-equivalent ellipsoid can effectively solve the problem in convergence.

(2) The morphology-equivalent ellipsoid is generated by considering the volume, shape factors and principal orientations of the real shrinkage. It can be found from the simulation results that using the morphology-equivalent ellipsoid is proved to have better prediction results than the volume-equivalent sphere.

(3) The volume-equivalent sphere underestimates the real closure degree during HIP which may be ascribed to the tortuosity of the surface of real shrinkage. The morphology-equivalent ellipsoid
underestimates slightly the real closure degree. It is inferred that some of the initial morphology must be favorable to void closure.

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