Effect of thermal behavior on the grain morphology and dimension of 80-mm-thick Ti6Al4V plates joined by laser melting deposition

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Abstract
As the material experiences non-uniform thermal expansion and contraction under different thermal behavior during laser melting deposition (LMD), the microstructure of the components will be affected, which also causes changes in mechanical properties. It is essential to understand the thermal behavior of the melt pool during LMD to improve the microstructure and joint quality. In this study, two 80-mm-thick Ti6Al4V plates are successfully joined using three different scanning speeds (10, 15, and 20 mm/s). The effects of thermal behavior on the grain morphology and dimension of deposition area, equiaxed crystal zone (EQZ), and the substrate at different scanning speeds are quantitatively analyzed. The results show that the fine equiaxed crystals are formed near the joint boundary due to the high-temperature gradient and cooling rate. The growth direction of fine columnar crystals continuously changes from the joint boundary to the center of the deposition area due to the change of heat-extraction direction. However, the epitaxial growth direction of the coarse columnar crystal is the same as the previous deposition layer at the center of the deposition area. Given the effect of high heat accumulation and low-temperature gradient during LMD, the dimension of columnar crystal is coarsen significantly at the center of the deposition area.

Keywords Laser melting deposition · Titanium alloy · Grain morphology · Grain dimension · Thermal behavior

1 Introduction

It is widely acknowledged that the welding method was widely and successfully used to join large-scale structures in some industrial fields such as aviation manufacture, power plants, shipbuilding, and pipelines manufacture [1]. High-quality welded joints have been achieved using multi-pass arc welding technology in the case of thicker plates (about 140–180 mm) used in pressure vessels [2]. However, considerable heat input and long cycle time of multi-pass arc welding technology give significant residual stresses and accompanied post-weld distortions [3].

In contrast to conventional processing methods such as multi-layer and multi-pass welding, laser welding with metal powder (LWMP) has unique and obvious advantages, including a high-intensity heat source, low heat distortion, small heat affected area, fast processing efficiency, and good metallurgical bonding [4–10]. Most of the previous research on LWMP processes mainly concentrates on the influence of the filler material on the microstructure and the mechanical properties of the joint [11–16]. However, LWMP is only applied to join thin plates with thick of 1 ~ 5 mm at present. In addition, there are some researches for joining titanium alloy or steel plates between 5 and 80 mm using electron beam welding [17–19] and laser welding with filler wire [1–3, 20]. However, a low volume of vacuum room or chamber is difficult to joining large-scale structures for electron beam welding, and the gap tolerance for the weld joint is too small. Meanwhile, the angle distortion of the base metal is easy to occur because of high heat input in laser welding with filler wire.

Large and complex components were fabricated layer-by-layer through laser melting deposition (LMD), a near-net-shape additive manufacturing process [21–24]. Compared with conventional processing methods such as forging or welding, LMD technology has the unique advantage of producing and joining large-scale components [25]. Typical applications of LMD include surface modification, repair of metallic
components, and connection of large-scale parts in automobile, aerospace, and ship domains. In the process of LMD, the joint quality depends on the thermal behavior and the LMD parameters such as spot size, focal position, laser power, and scanning speed. Therefore, joining large-scale substrates’ critical problem is controlling thermal behavior, which establishes a cardinal relationship between microstructure and mechanical property and dictates the joint performance.

Sun et al. [26] utilized a coaxial imaging system to observe the real-time pool characteristics in the process of LMD. The morphology of the melt pool and the cross-sectional dimension of the solidified track and grain structures of the solidified tracks were predicted under different heat inputs. Zhan et al. [27] quantitatively analyzed the microstructure and associated thermal process to explore the microcosmic mechanism during the LMD process using an Invar alloy. Subsequently, the relationship between the microstructure and thermal conditions was established using simulation and experimental work. Xiang et al. [28] applied LMD to the fabrication of CrMnFeCoNi high entropy alloys. It was reported that laser power and scanning speed significantly impact CET transitions in the top region of LMD processed samples due to the effect of these parameters on heat flux direction and temperature gradient. Xu et al. [29] investigated the effect of heat input, especially by altering the laser scanning speed, on phase composition, microstructure, microhardness, residual stresses, and tensile properties of the specimens. The average granular size was refined as the laser scanning speed increased. In addition, LMD processed 12CrNi2 alloy steel can meet the requirements of low alloy steel components due to its sufficient strength and toughness.

Ti6Al4V is considered the “main force” of titanium alloys due to its high specific strength, good corrosion resistance, and high toughness, which is widely and successfully used in the marine and aerospace industry [30–33]. Due to the large temperature gradient and rapid solidification rate during LMD, Ti6Al4V alloys are typically characterized by large columnar grains with ultrafine basket-weave microstructure, which is beneficial to mechanical properties [34–37]. To cope with the challenges associated with joining large-scale titanium alloy components primarily used in the automotive industry, satellite launch vehicles, and aircraft gas turbine engines, it seems pertinent to introduce LMD technology that can conveniently fabricate large-scale components by layer. However, the research results on the joining process of large-scale titanium components processed by LMD and whose thickness is around 80 mm are rarely reported.

The objective of the present research is to use LMD as a method for joining the 80-mm-thick Ti6Al4V plates to explore the morphology evolution of grains from deposition area to substrate under different thermal behavior. The change of grain dimension in deposition area, EQZ, heat affect zone (HAZ), and substrate with different heat input decided by scanning speed is quantitatively measured and analyzed. The effect of temperature gradient and solidification on grain morphology is discussed. The laser holding time and scanning speed are applied to estimate the grain dimension. The growth direction of columnar crystals under the different orientations of radiation is explored.

Therefore, a research plan has been executed by exploiting Ti6Al4V titanium alloy (80 mm) as a substrate and processed using LMD. The investigation has been done using different scanning speeds to understand the thermal distribution and its subsequent effect on microstructure evolution. The morphology and scale of the grain structure, both in the vicinity of joint boundary and in the central region of deposition area, have been quantitatively analyzed and explained in the light of temperature distribution. In sum, LMD is an ideal method to realize large-scale joining parts such as frame and beam structure in aircraft, conducive to improving joint quality and speed up production efficiency. Our research will pave the way for microstructure regulation and the adjustment of mechanical properties in various regions in large-scale components jointing by LMD. Meanwhile, the influence mechanism of thermal behavior on the grain morphology should be revealed to solve the problem of uneven microstructure and properties from joint boundary to the center of deposition area. It also provides theoretical guidance for manufacturing large-scale parts in the aviation and spaceflight area.

### 2 Materials and methods

Powder particles of Ti6Al4V having a spherical shape and diameter in the range of 80–150 μm were fabricated using a plasma rotating electrode process (PREP). Chemical composition of the powder is shown in Table 1. Dehumidification process was executed in a vacuum furnace within which the temperature was maintained at 102 °C for 2 h. Subsequently, the furnace was cooled to room temperature under the condition of vacuum after the insulation. Ti6Al4V base plates were first cut by electrical discharge machine (EDM). After cutting, they were prepared on the milling machine to ensure the flatness and parallelism of the faying surfaces. Figure 1a, b demonstrate the configuration and detailed joint design dimensions. Before the LMD experiment, the faying surfaces were polished with coarser sandpaper to remove the surface oxide layer and washed with acetone.

| Element | Al  | V   | Fe  | C   | N   | H   | O   | Ti   |
|---------|-----|-----|-----|-----|-----|-----|-----|------|
| Composition (wt%) | 5.5–6.8 | 3.5–4.5 | 0.30 | 0.10 | 0.05 | 0.015 | 0.20 | Bal. |
LMD system for a current experiment comprises a 10-kW fiber laser system, argon chamber, powder feeding system with a coaxial nozzle, a motion system utilizing 5-axis CNC machine tools, and a cooling water system shown in Fig. 2. The laser beam emitted from the end of the fiber, and the measured focus spot diameter was 3 mm. A coaxial nozzle was connected to the powder feeder with a tube, and powder was delivered into the molten pool by coaxial nozzles, which were 15–20 mm above the substrate. The coaxial nozzle was mounted on a 5-axis CNC machine tool. LMD joins the 80-mm-thick Ti6Al4V plates in an Argon chamber purged with high purity argon. Before an experiment, the argon chamber of the LMD system was cleaned and a vacuum degree below $5.0 \times 10^{-2}$ Pa was achieved. Afterward, high purity inert gas argon was filled into the chamber, which ensured the oxygen concentration in the deposition chamber to be less than 50 ppm.

The molten pool was formed by irradiating the laser beam on the surface of the substrate. At the same time, the Ti6Al4V powder was introduced into the molten pool at a high temperature through the powder feeding nozzle under the restriction of the powder gas. The Ti6Al4V powder melted quickly after entering the molten pool to deposit successive layers between the two Ti6Al4V plates, as is shown in Fig. 1a, b. As the laser beam traversed, solidification of the molten pool was initiated in the trailing half of the molten pool on the surface of the previously deposited layer. Because of this multi-pass process, HAZ was also created in the already deposition layer by heat conduction. The overall schematic of this process is shown in Fig. 1c. The X-shaped groove was filled layer by layer with an overlap ratio of 50% till the top surface of two Ti6Al4V plates. Processing parameters of LMD are listed in Table 2.
In order to explore microstructural attributes, samples were extracted from the joint boundary to the central region of the deposition area. These samples were ground with progressively increasing abrasive papers up to 2000# and then polished with a diamond abrading agent having a particle size of 1 µm. After that, these samples

| Laser power (W) | Scanning velocity (mm/s) | Powder feeding rate (g/min) | Shielding gas flow (L/min) | Spot diameter (mm) | Overlap ratio (%) | Increment of Z (mm) |
|----------------|--------------------------|-----------------------------|---------------------------|-------------------|------------------|--------------------|
| 1500           | 10, 15, 20               | 8                           | 4                         | 3                 | 50               | 0.7 – 1.5          |
were etched by the Kroll reagent (4 mL HNO₃ + 2 mL HF + 100 mL H₂O). Grain structure was recorded by the stereomicroscope, which analyzed the apparent grain morphology and characteristic scale evolution between the joint boundary and the center of deposition area. In addition, the grain dimension transformation in the different regions was analyzed and contrasted under different scanning speeds.

3 Results and discussion

3.1 Relationship between grain morphology and temperature distribution

Figure 3 shows the influence of thermal behavior on the macromorphology of the LMD joint when the laser power is 1500 W and the scanning speed is 10 mm/s. An equiaxed crystal zone (EQZ) is observed near the joint boundary in Fig. 3b and the average width of EQZ is 2.06 mm in Fig. 3d. Quantitative characterization of the average size of an equiaxed crystal in EQZ is done through measuring software. The distribution of grain diameters shows the normal distribution, and the average grain diameter is 0.27 mm, as shown in Fig. 3e. After that, the epitaxial growth of fine columnar crystal occurs by the evident phenomenon of heterogeneous nucleation aided by already existing equiaxed crystals, as shown in Fig. 3b. The sidewall of the joint boundary is peculiarly prone to conduct heat rapidly, inducing a rapid increase of undercooling degree for nucleation. It could be explained by the fact that the relatively higher undercooling degree promotes nucleation rate, leading to the formation of more refined grain near the sidewall of the X-shaped groove. However, columnar crystals coarsen significantly at the middle deposition layer of the X-shaped groove. It can be speculated that the phenomenon of heat accumulation at
the middle deposition layer of X-shaped groove facilitates the growth of coarser columnar crystal shown in Fig. 3c.

The finite element model is established to calculate the temperature field distribution in the local process of LMD. Details of the shape of molten pool and laser energy density of Gauss heat source during LMD process are shown in Fig. 4a, b. In Fig. 4b, it is found that the maximum value of energy density of the laser beam can reach $2.12 \times 10^7$ W/m$^2$.

The general expression for the energy density distribution $q$ is calculated as follows:

$$ q = \alpha_p \cdot P \cdot \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-x_0)^2}{2\sigma^2}} \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(y-y_0)^2}{2\sigma^2}} $$

(1)

where $\alpha_p$ is powder absorptivity, $P$ is the laser power, and $\sigma$ is the Gaussian distribution function taken as a quarter of the laser spot diameter. The laser spot diameter is 3 mm in this experiment. Initial location of the coordinate system is given by $x_0$ and $y_0$, while the main field spatial variables are $x$ and $y$. During LMD process, the deposition powder and surface of substrates are melted. The surface of substrates forms an ellipsoidal shape molten pool under the effect of Gaussian heat source distribution. The elongated shape of the molten pool could be attributed to the higher laser scanning speed, as shown in Fig. 4a.

The heat conduction process of substrate occurs after laser irradiation, which can be described by Eq. (2) [27]:

$$ \rho C_p \frac{\partial T}{\partial \tau} = \left[ \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \lambda \frac{\partial T}{\partial z} \right) \right] + Q $$

(2)

where $\rho$ is the density of Ti6Al4V plates, which is about 4.5 g/cm$^3$. The specific heat ($C_p$) is measured at 0.52 J/(kg·°C). The thermal conductivity ($\lambda$) reaches 15.24 W/(m·K), and $Q$ stands for the internal heat source. Besides, initial conditions have been set according to the experimental conditions including initial temperature of the substrate and powder. Therefore, initial temperature of the substrate and powder are set to 25 °C. Meanwhile, the LMD process adopts the boundary conditions considering the convective heat transfer between deposition layer, substrates, and environment, as described in Eq. (3) [27]:

$$ q' = -h(T - T_0) $$

(3)

where $q'$ is the energy density distribution on the boundary and $h$ is the heat transfer coefficient, which can reach 6 W/(m$^2$·K) through experiment measurement. $T$ is the transient temperature of powder and substrate during LMD. $T_0$ is the temperature of environment, which is also set to 25 °C.

Figure 4c shows the temperature distribution curve around the molten pool when the laser power is 1500 W and the scanning speed is 10 mm/s through solving the above finite element model. The model created the process...
of single-track laser melting at the surface of substrates, which explains the evolution of grain morphology and dimension at the LMD joint under temperature distribution. The temperature in the center of molten pool (Node 1) is about 2004.68 °C. As the distance from the center of the molten pool increasing to 0.2 mm, the temperature reduces to 1515.52 °C at Node 2. In addition, the temperature around the HAZ changes from 883.30 (Node 3) to 475.88 °C (Node 4), which lies in the range between 0.5 and 1.0 mm from the center of molten pool. Therefore, sharp temperature gradients give rise to higher undercooling levels in the vicinity of HAZ, thus facilitating the conditions for the formation of refined grains around the joint boundary. Then sharp temperature gradients give rise to higher undercooling levels in the vicinity of HAZ, thus facilitating the conditions for forming refined grains around the joint boundary. However, coarser columnar crystals are formed easily after the solidification of the molten pool because of the low-temperature gradient and undercooling level at the center of the deposition area. Finally, at a distance exceeding 3 mm from the molten pool center, the temperature remains at 25 °C (Node 5).

The process of grain morphology transition from the β-equiaxed crystal at EQZ to the β-columnar crystal at the LMD joint is presented in Fig. 5a. Both nucleation rate (N) and growth rate (G) of the grains are generally considered as being proportional to the undercooling level, which decreases as the S/L interface advances towards the central region of the molten pool [38]. However, the value of N/G of grains is less than 1 (N/G < 1) at the center of the deposition area, which reduces the number of grains per unit volume Zv. The relationship between Zv and N/G is depicted by Eq. (4) [39].

\[
Z_v = 0.9 \left( \frac{N}{G} \right)^{\frac{1}{4}}
\]

When the value of N/G of grains exceeds 1 (N/G > 1), columnar crystals tend to be finer as the undercooling is high close to the joint boundary. In addition, a large number of fine equiaxed crystals are formed at EQZ due to a high undercooling degree when the value of nucleation rate (N) far exceeds growth rate (G).

Figure 5b shows that the “component supercooling” zone starts to appear when the actual temperature gradient
of equiaxed crystal follows a normal distribution in EQZ. The peak value of the Gaussian distribution curve is shifted to the left, which indicates that the average grain diameter of the equiaxed crystal goes down as the scanning speed increases, as revealed in Figs. 3c and 6c, g. Specifically, the average grain diameter is about 0.27 mm when the laser power is 1500 W and the scanning speed is 10 mm/s. As the scanning speed is increased up to 15 and 20 mm/s, the average grain diameter goes down to 0.21 and 0.18 mm because of an apparent reduction in heat input. A similar trend can be observed in the microstructural morphology in the central region, as displayed in Fig. 6b, f. It can be noticed that the aspect ratio of columnar crystals decreases as the speed is increased from 15 to 20 mm/s.

Figure 7 confirms that the influence of scanning speed on the dimension of fine columnar crystals at the joint boundary. With the scanning speed increasing from 10 to 20 mm/s, the length of the fine columnar crystals decreases from 1.02 to 0.55 mm due to a noticeable reduction in local heat input and concomitant increase in cooling rate. However, scanning speed has no significant impact on fine columnar crystals’ width, which always keeps stable at about 0.21 mm. The width of coarse columnar crystals at the central region demonstrated a continuous downward trend as the speed was increased from 10 to 20 mm/s in Fig. 8b. The average width of coarse columnar crystal is 1.03 for 10 mm/s, which is quite similar to the width of fine columnar crystal in the vicinity of joint boundary (see Fig. 8c). However, the width of coarse columnar crystal is reduced by 17.5% when the scanning speed is increased to 15 mm/s (see Fig. 8d). The most significant reduction of more than 50% in the width of coarse columnar crystals is achieved with a speed of 20 mm/s, as shown in Fig. 8e. However, the exact length of coarse columnar crystals is difficult to obtain because the view goes beyond the range of stereomicroscope.

There is a special relationship between the temperature of molten pool and laser scanning speed during the process of LMD. The analytical expression of the temperature of molten pool can be summarized as follows [40]:

$$T(r, x) = \frac{AP}{2\pi kr} \exp\left(-\frac{Vr}{2a} - \frac{Vx}{2a}\right)$$

where A is the absorption coefficient because feeding power can absorb part of laser, P is the laser power, k is the thermal conductivity, α is the thermal diffusivity, r is the distance between the origin of the moving coordinate and the calculation point, x is coordinates of calculation points, and V is the laser scanning speed. Therefore, it can be identified the
The temperature of molten pool $T(r,x)$ is rising with the laser scanning speed $V$ decreasing.

In order to explore grain growth kinetics of fine columnar crystal near the joint boundary during LMD process, a classical grain growth kinetics equation was used [41]:

$$G^n - G_0^n = K_0 t \exp \left( -\frac{Q}{RT} \right)$$

(7)

where $G$ is the average grain dimension of columnar crystal, $G_0$ is the grain size of substrate, $n$ is the grain growth kinetic exponent, $K_0$ is a constant, $t$ is the holding time of laser at a position, $R$ is an ideal gas constant at 8.314 J/(mol·K), $T$ is absolute temperature, and $Q$ is the grain growth activation energy. Due to the larger dimension of grain in deposition than that in the substrate ($G \gg G_0$), $G_0$ can be neglected. Therefore, Eq. (8) can be simplified as

$$\lg G = \frac{1}{n} \lg t + \frac{1}{n} \left( \lg K_0 - 0.434 \frac{Q}{RT} \right)$$

(8)

When the laser scanning speed increases, the laser holding time $t$ is shortened, and the average grain dimension of columnar crystal decreases according to Eq. (8).
Moreover, when the holding time $t$ is constant, Eq. (9) can be simplified as

$$
\lg \frac{G'_{\text{m}}}{G_{\text{m}}} = \left(-0.434 \frac{Q}{K}\right) T^{-1} + \lg K_0
$$

According to Eq. (7), the grain dimension of columnar crystal $G$ rises when the laser holding time is prolonged, which means the laser scanning speed is low.

In addition, the dimension of columnar crystal is coarser in the center of the deposition layer due to heat accumulation. The large columnar grains continue to grow during solidification because the temperature gradient and cooling rate are low. The growth direction of coarse columnar crystal is determined by the heat-extraction direction ($Q_v$), which is perpendicular to the molten-pool profile, as is shown in Fig. 9a. The fine columnar crystals are grown along with the orientation of radiation ($Q_v$) which is perpendicular to the sidewalls of the X-shaped groove. Curved growth of fine columnar crystal can also take place shown in Fig. 9b. It can be explained that the growth direction of fine columnar crystals is perpendicular to the X-shaped groove’s sidewall, which grows along the opposite direction of heat dissipation. After that, the fine columnar crystal changes to another growth direction which is perpendicular to the molten-pool profile. Therefore, the curved growth of fine columnar crystals is relevant to radiation orientation ($Q_v$).

For the curved growth phenomenon, the orientation angle has already changed because of the different directions of the molten-pool profile and $Q_v$ between the joint boundary and the center of the deposition layer [39]. However, the orientation angle of the epitaxial growth of the coarse columnar crystal is the same as that of the previous deposition layer in the center of the deposition area shown in Fig. 9c. The direction of $Q_v$ is always perpendicular to the horizontal plane. The epitaxial growth of coarse columnar crystal along straight lines is induced by the direction of $Q_v$ in the center of the deposition area.
Fig. 8 Quantitative measurement of coarse columnar crystal dimension with different scanning speeds in the center of deposition area. (a) Macro morphology of LMD joint depicting areas with different scanning speeds; (b) variation of the width of coarse columnar crystal with relevant scanning speed; (c) the macro morphology of coarse columnar crystal with the scanning speed at 10 mm/s; (d) the macro morphology of coarse columnar crystal with the scanning speed at 15 mm/s; (e) the macro morphology of coarse columnar crystal with the scanning speed at 20 mm/s.

Fig. 9 Schematic diagram of columnar crystal growth for Ti6Al4V thick plates in the process of LMD. (a) Grain morphology and its growth direction in different regions; (b) curved growth of columnar crystals at the joint boundary; (c) epitaxial growth of columnar crystals at the center of deposition area.
4 Conclusions

In the present study, Ti6Al4V titanium alloy thick plates (80 mm) have been joined through an LMD method by adopting different laser scanning speeds. The micromorphology of grains about different local heat distribution due to varying heat input has been investigated. The main findings can be summarized as follows:

1. Equiaxed crystal is formed in the EQZ near the joint boundary because of the high undercooling level. Epitaxial growth of fine columnar crystals grows on the equiaxed crystals in the process of LMD. The fine columnar crystal becomes coarser significantly at the center of the deposition area due to heat accumulation, located at the middle deposition layer of the X-shaped groove. It can be seen that there is different temperature distribution in different positions on the Ti6Al4V plates, which accounts for different grain morphology.

2. Quantitative measurement of the equiaxed crystal size and the width of the equiaxed crystal zone at different scanning speeds was executed by commercial software. The average grain diameter of equiaxed crystal follows a normal distribution in the equiaxed crystal zone. As the scanning speed is increased, the average grain diameter declines slightly because of the decrease of heat input during LMD operation.

3. Quantitative measurement of the length and width of fine columnar crystal at the joint boundary revealed an inverse relationship with the scanning speed, which causes a decrease in the heat input decreasing and an increase in cooling rate. However, scanning speed has no significant effects on the width of fine columnar crystals. Meanwhile, the width of coarse columnar crystal in the center of the deposition area is reduced by 17.5%, with the scanning speed rising from 10 to 15 mm/s. When the scanning speed continues to increase to 20 mm/s, the width reduction of coarse columnar crystal is more than 50%.

4. Due to the effect of undercooling levels in different regions of the LMD joint, a large number of fine equiaxed crystals are formed in EQZ. A fine columnar crystal grows epitaxially from the fine equiaxed crystals in EQZ. Then the fine columnar crystal changes another direction continuing to grow along the direction of \( Q \), which is perpendicular to the molten-pool profile. However, at the center of the deposition area, the ratio of nucleation rate and growth rate is negative, which means the coarse columnar crystals can be formed in this region, and the orientation angle of epitaxial growth of the coarse columnar crystals are same as before at the center of deposition area.

Author contribution Feiyue Lyu: investigation, data curation, formal analysis, writing — original draft. Ke Hu: methodology, writing — review and editing. Leilei Wang: writing — review and editing, validation. Feng Yu: resources, data curation. Xiaohong Zhan: conceptualization, supervision.

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Availability of data and material The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of an ongoing study.

Declarations

Conflict of interest The authors declare no competing interests.

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