

Evolution equations of deformation twins in metals—Evolution of deformation twins in pure titanium

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Abstract

The evolution equations of the volume fractions of deformation twins are obtained in this article by using the theory of inclusions in micromechanics and analyzing the Gibbs free energy and dissipation of a system. The evolution process of the volume fractions of twins is got by using the Runge–Kutta method in this article. The computational results of the evolution equations (the critical twinning stress and the families of twins appeared under different loading conditions) are consistent with the experiment results.

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1. Introduction

Twinning is an important mode of plastic deformation in FCC metals of low stacking-fault energy (e.g. α -brass, MP35N) and most of HCP metals (e.g. α -Ti, Zr). Recently, more and more researchers have realized that twinning has important influence on the plastic deformation of these metals [1–3]. Ayman et al. [3] associated the three distinct stages of strain hardening of α -Ti deformed under uniaxial compression with deformation twinning. A mesoscopic constitutive model of Hadfield steel was proposed by Karaman et al. [4], based on the relationship between the resistance of the motion of dislocations and the volume fractions of deformation twins. Researchers have also realized that deformation twinning plays an important role in the texture evolution of these metals. The influence of deformation twinning on texture evolution of Zr has been simulated by Tome et al. [5]. In order to learn more about the twinning, Yoo and others [6,7] discussed the elastic energy caused by deformation twins by using the theory of inclusions and proposed the possible reasons of the appearance of different types of deformation twins at

different temperature under a certain mode of load. Lebensohn and Tome [8] and Meyers et al. [9] obtained the relationship between the critical stress of deformation twinning and the shapes and sizes of twins by using theory of inclusions within the scope of thermomechanics. However, they have not got the critical stress of deformation twinning and the evolution of deformation twinning after the appearance of twins. In this paper, we try to establish the evolution equations of the volume fractions of deformation twins in metals by analyzing the Gibbs free energy of a system and using the theory of inclusions in micromechanics.

2. Modeling the evolution of the volume fractions of deformation twins

2.1. Representative volume element (RVE)

In Fig. 1, the blank represents the plastic–elastic matrix and the shadow represents twins, which are regarded as elastic inclusions because of their small thickness [10]. The eigenstrain of the inclusions could be deduced from small strain analysis as follows:

$$\epsilon_{ij}^t = \frac{1}{2}s(n_i m_j + n_j m_i), \quad (1)$$

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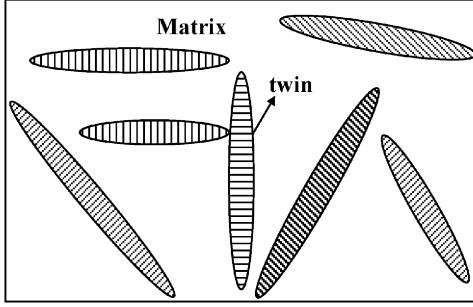


Fig. 1. Representative volume element.

where s denotes the magnitude of twinning shear, n , m denote the direction of twinning shear and the normal direction of the shear plane, respectively.

A large number of experiments showed that twins often appear in lenticular shapes. For simplicity, the shape of twins is assumed to satisfy the equation of ellipsoids

$$x_1^2/a^2 + x_2^2/a^2 + x_3^2/(\mu a)^2 = 1 \quad (\mu \ll 1). \quad (2)$$

Short axis is perpendicular to the shear plane and the long axis is parallel to the direction of twinning shear.

2.2. Thermomechanical analysis of the evolution of the deformation twins

The complementary free energy of a system is defined by

$$\psi(\Sigma, f_i) = -(\phi(\Sigma, f_i) - \Sigma : E), \quad (3)$$

where f_i denotes the volume fractions of deformation twins of the i th type. Σ , E denote the volume averaged stress and volume averaged strain, respectively,

$$\Sigma = \frac{1}{V} \int_V \sigma \, dV, \quad E = \frac{1}{V} \int_V \epsilon \, dV. \quad (4)$$

ϕ denotes the Helmholtz free energy of the system,

$$\phi(\Sigma, f_i) = W_{\text{elastic}} + \Gamma_{\text{interface}} + W_{\text{chem}}, \quad (5)$$

where W_{elastic} denotes the elastic energy of the element, $\Gamma_{\text{interface}}$ denotes the interface energy of twins and W_{chem} denotes the chemical free energy of the system.

2.2.1. Elastic energy of the element

The elastic energy of the RVE is [11]

$$W_{\text{elastic}} = \frac{1}{2} \Sigma : M : \Sigma - \sum_{i=1}^N \frac{1}{2v_i} \int_{v_i} \langle \sigma \rangle : \epsilon^t \, dv_i, \quad (6)$$

where M denotes the compliant tensor of matrix, v_i denotes the volume of the deformation twins of i th type, N denotes the number of the type of twins.

Under load $\bar{\epsilon}_p$ is assumed to be the homogeneous plastic strain of matrix. According to the Mori–Tanaka self-consistent theory, the volume averaged stress could

be obtained

$$\begin{aligned} \langle \sigma \rangle_i &= L : (S_i - I) : (\epsilon_i^t - \bar{\epsilon}_p) \\ &- L : \sum_{s=1}^N (S_s - I) : (\epsilon_s^t - \bar{\epsilon}_p) f_s, \end{aligned} \quad (7)$$

where S_i denotes the Eshelby tensor of the twins of i th type.

$$\begin{aligned} W_{\text{elastic}} &= \frac{1}{2} \Sigma : M : \Sigma \\ &- \frac{1}{2} \sum_{i=1}^N f_i (\epsilon_i^t - \bar{\epsilon}_p) : L : (S_i - I) : \epsilon_i^t \\ &+ \frac{1}{2} \sum_{i=1}^N \sum_{s=1}^N f_i f_s (\epsilon_i^t - \bar{\epsilon}_p) : L : (S_s - I) : \epsilon_s^t, \end{aligned} \quad (8)$$

where the third term reflects the interaction of different types of twins [11].

2.2.2. Complementary free energy of the element

According to Eq. (3), the volume averaged stress and volume averaged strain could be expressed as

$$\Sigma = \sum_{i=1}^N f_i \langle \sigma \rangle_{v_i} + (1-f) \langle \sigma \rangle_{v_m}, \quad f = \sum_{i=1}^N f_i, \quad (9)$$

$$E = \langle \epsilon^e \rangle_v + \langle \epsilon^p \rangle_v = M : \Sigma + \sum_{i=1}^N f_i \epsilon_i^t. \quad (10)$$

Because the time needed for a twin plate growing from nucleation the ultimate size is much shorter than the characteristic time of the increase of the volume fractions of twins [12], the increase of the volume fractions of twins could be simply considered as the increase of the numbers of the twin plates, and the interface energy of twins per volume can be expressed as

$$\Gamma_{\text{interface}} \approx \sum_{i=1}^N \frac{3\gamma_i}{2a_i\mu_i} f_i, \quad (11)$$

where a_i is a constant, which reflects the size of a twin plate.

Substituting Eqs. (8)–(11) into Eq. (3), we obtain

$$\begin{aligned} \Psi(\Sigma, f_i) &= \frac{1}{2} \Sigma : M : \Sigma \\ &+ \Sigma : \left[\sum_{i=1}^N \epsilon_i^t f_i + \left(1 - \sum_{i=1}^N f_i \right) \bar{\epsilon}_p \right] \\ &+ \frac{1}{2} \sum_{i=1}^N f_i (\epsilon_i^t - \bar{\epsilon}_p) : L : (S_i - I) : \epsilon_i^t \\ &- \frac{1}{2} \sum_{i=1}^N \sum_{s=1}^N f_i f_s (\epsilon_i^t - \bar{\epsilon}_p) : L : (S_s - I) : \epsilon_s^t \\ &- \sum_{i=1}^N \frac{3\gamma_i}{2a_i\mu_i} f_i - W_{\text{chem}}. \end{aligned} \quad (12)$$

2.2.3. Evolution of volume fractions of deformation twins

According to thermomechanical theory, the increase of complementary free energy of a system is equal to dissipative energy of the system

$$d\psi|_{\Sigma,T} = dW_d \geq 0. \tag{13}$$

Based on the internal variable theory, the driving force of twinning can be expressed as

$$\begin{aligned} \tau_i &= \frac{\partial \dot{W}_d}{\partial \dot{f}_i} = \Sigma : (\epsilon'_i - \bar{\epsilon}_p) \\ &+ \frac{1}{2}(\epsilon'_i - \bar{\epsilon}_p) : L : (S_i - I) : \epsilon'_i \\ &- \sum_{s=1}^N f_s (\epsilon'_s - \bar{\epsilon}_p) : L : (S_s - I) : \epsilon'_i - \frac{3\gamma_i}{2a_i\mu_i}. \end{aligned} \tag{14}$$

It is assumed in this article that when the driving force of twinning $\tau_i \geq \tau_c$, $k\dot{f}_i = (\tau_i - \tau_c)$ i.e.

$$\begin{aligned} k \frac{df_i}{dt} &= \Sigma : (\epsilon'_i - \bar{\epsilon}_p) + \frac{1}{2}(\epsilon'_i - \bar{\epsilon}_p) : L : (S_i - I) : \epsilon'_i \\ &- \sum_{s=1}^N f_s (\epsilon'_s - \bar{\epsilon}_p) : L : (S_s - I) : \epsilon'_i \\ &- \frac{3\gamma_i}{2a_i\mu_i} - \tau_c \quad \text{when} \quad \tau_i \geq \tau_c. \end{aligned} \tag{15}$$

A large number of experiment results show that the de-twinning does not occur during plastic deformation, i.e.

$$\frac{df_i}{dt} \geq 0 \tag{16}$$

and f_i should also satisfy

$$f_i \geq 0, \quad \sum_{i=1}^N f_i \leq 1. \tag{17}$$

Eqs. (15)–(17) are the equations of evolution of volume fractions of deformation twins.

When $(df_i/dt) = 0$ (the driving force of twinning τ_i reach the critical value τ_c), Eq. (15) can be reduced to the equations of the critical twinning stress:

$$\begin{aligned} \Sigma : (\epsilon'_i - \bar{\epsilon}_p) + \frac{1}{2}(\epsilon'_i - \bar{\epsilon}_p) : L : (S_i - I) : \epsilon'_i \\ - \sum_{s=1}^N f_s (\epsilon'_s - \bar{\epsilon}_p) : L : (S_s - I) : \epsilon'_i \\ - \frac{3\gamma_i}{2a_i\mu_i} - \tau_c = 0. \end{aligned} \tag{18}$$

Based on the shape parameters, directions, magnitude of shear and interface energy of twins and the elastic constants of materials, the equations of evolution of volume fractions of deformation twins could be solved by

Table 1
Parameters of deformation twins of titanium adopted in this work

Twins family	Type	n1	n2	n3	m1	m2	m3	S	Interface energy of twins (mJ/m ²)
(10 $\bar{1}$ 2)	1	-0.737	0	0.676	0.676	0	0.737	0.174	292
	2	-0.369	-0.639	0.676	0.338	0.585	0.737		
	3	0.369	-0.639	0.676	-0.338	0.585	0.737		
	4	0.737	0	0.676	-0.676	0	0.737		
	5	0.369	0.639	0.676	-0.338	-0.585	0.737		
	6	-0.369	0.639	0.676	0.338	-0.585	0.737		
(2 $\bar{1}$ $\bar{1}$ 2)	7	0.462	-0.267	-0.846	0.733	-0.423	0.533	0.219	266
	8	0.462	0.267	-0.846	0.733	0.423	0.533		
	9	-0.463	0.267	-0.846	-0.733	0.423	0.533		
	10	-0.462	-0.267	-0.846	-0.733	-0.423	0.533		
	11	0	0.533	-0.846	0	0.846	0.533		
	12	0	-0.533	-0.846	0	-0.846	0.533		
(11 $\bar{2}$ 1)	13	-0.260	0.150	0.954	0.826	-0.477	0.300	0.63	212
	14	-0.260	-0.150	0.954	0.826	0.477	0.300		
	15	0.260	-0.150	0.954	-0.826	0.477	0.300		
	16	0.260	0.150	0.954	-0.826	-0.477	0.300		
	17	0	-0.301	0.954	0	0.954	0.300		
	18	0	0.301	0.954	0	-0.954	0.300		
(10 $\bar{1}$ 1)	19	0.479	0	-0.878	0.878	0	0.479	0.099	765
	20	0.240	0.415	-0.878	0.439	0.760	0.479		
	21	-0.240	0.415	-0.878	-0.439	0.760	0.479		
	22	-0.479	0	-0.878	-0.888	0	0.479		
	23	-0.240	-0.415	-0.878	-0.439	-0.760	0.479		
	24	0.240	-0.415	-0.878	0.439	-0.760	0.479		

using proper numerical methods, and the evolution process could also be obtained.

3. Numerical results of the evolution of the volume fractions of deformation twins in single crystal α -titanium

The Runge–Kutta method is adopted to solve the evolution equations in this article. The magnitude of twinning shear, s , and the direction of twinning shear and the normal direction of the plane of shear, n , m could be obtained from Ref. [8], see Table 1. The interface energy of deformation twins of titanium calculated by Yoo and Lee [7] is adopted in this article; also see Table 1.

According to three different tensile directions: (0.184, 0.0351, 0.982), (0.625, 0.0245, 0.780), (0.470, 0.169, 0.866), the numerical results of the evolution equations (the evolution process of deformation twins in pure titanium) is obtained. The numerical results is shown in Figs. 2(a)–(c) and Table 2, and the corresponding experimental results cited from Ref. [13] is also shown in Figs. 2(a)–(c) and Table 2.

Figs. 2(a)–(c) and Table 2 indicate:

- When $X_B = 78^\circ$ (X_B is the angle between the direction of load and C -axis of single crystal), the computed critical twinning stress is close to the experiment results got by Akhtar [13] (Table 2). When stress is lower than 400 Mpa, the type of deformation twins in titanium is mostly $(10\bar{1}2)$ (Fig. 2(a)), which is also consistent with experiment results.
- When $X_B = 47^\circ$, the computed critical twinning stress is also close to the experiment results got by Akhtar [13] (Table 2). And, the type of deformation twins is $(10\bar{1}2)$ and $(11\bar{2}1)$ (Fig. 2(b)), and the volume fractions of $(11\bar{2}1)$ is more than those of $(10\bar{1}2)$ all the time, which is consistent with the experiment results that the $(11\bar{2}1)$ twin is the primary type of deformation twin when $X_B = 47^\circ$.
- When $X_B = 60^\circ$, the computed critical twinning stress deviates from the experiment results got by Akhtar [13] (Table 2). And the volume fractions of $(10\bar{1}2)$ twins are almost equal to the volume fractions of $(11\bar{2}1)$ all the time (Fig. 2(c)), but when $X_B = 60^\circ$, $(11\bar{2}1)$ twins were only observed at low temperature (78 K) and $(10\bar{1}2)$ twins are only observed at high temperature (423 K) in experiments. There are two possible reasons about the divergence. Firstly, the influence of temperature on the interface energy of twins is neglected in this article (the interface energy of twins adopted in this article is computed by Yoo and Lee [7] at room temperature). Secondly, the difference between the nucleation stress of twinning and the initial stress needed to maintain the growth of the twins has not been taken into consider in this model. Actually, however, in most conditions, the nucleation stress, which is very hard to be precisely measured, is little higher than the initial stress needed to maintain the growth of the twins.

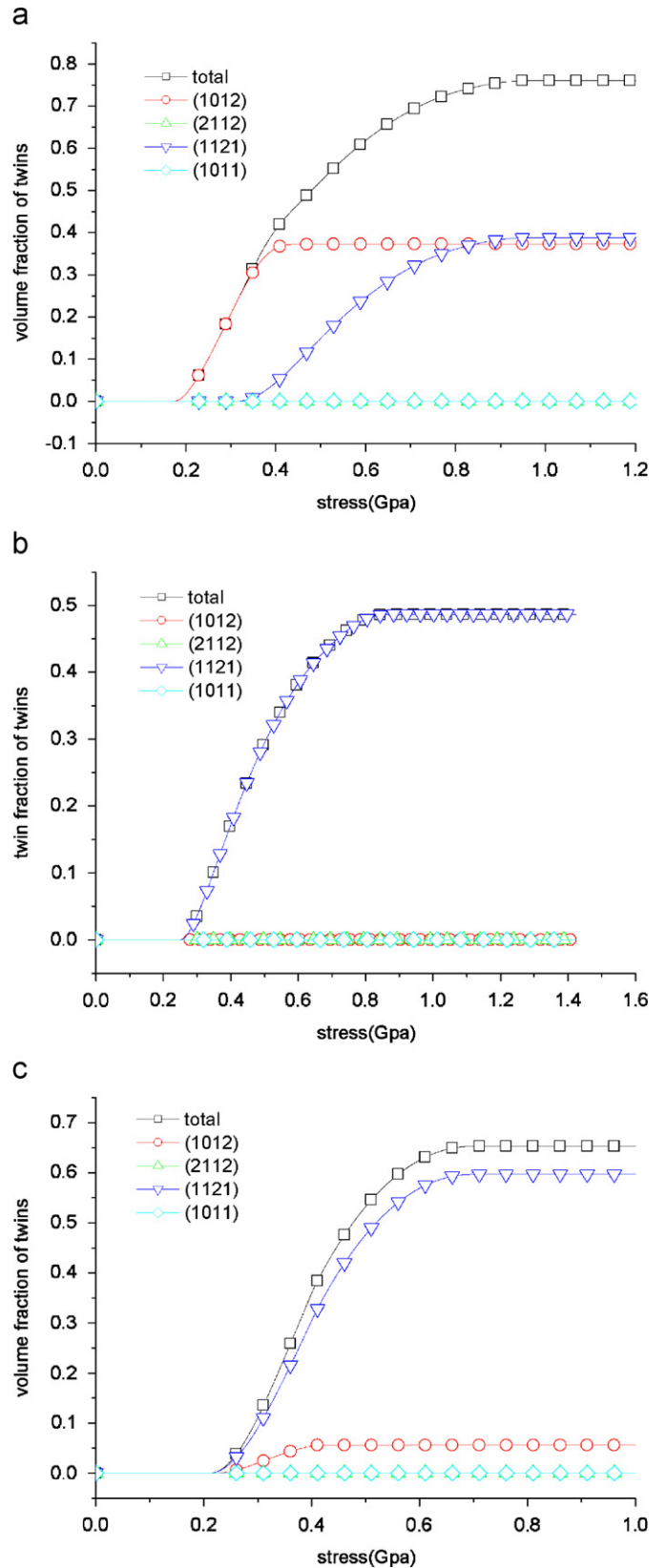


Fig. 2. Evolution of the volume fractions of deformation twins under tensile load at various directions. (a) $X_B = 78^\circ$; (b) $X_B = 47^\circ$; (c) $X_B = 60^\circ$.

Table 2
Predicted and observed critical twinning stress and twinning modes in titanium

Loading mode	Direction of loads	Experimental critical twinning stress (Mpa)	Types of twin observed in experiments	Computational critical twinning stress (Mpa)	Types of twin predicted by computation
<i>T</i>					
$X_B = 78^\circ$	(0.184, 0.0351, 0.982)	182	(10 $\bar{1}$ 2)	215	(11 $\bar{2}$ 1) (10 $\bar{1}$ 2)
$X_B = 47^\circ$	(0.625, 0.0245, 0.780)	170	(11 $\bar{2}$ 1)	208	(11 $\bar{2}$ 1) (10 $\bar{1}$ 2)
$X_B = 60^\circ$	(0.470, 0.169, 0.866)	390	(10 $\bar{1}$ 2) (78 K) (11 $\bar{2}$ 1) (423 K)	170 (78 K)	(10 $\bar{1}$ 2) (11 $\bar{2}$ 1)
<i>C</i>					
C-axis	(0,0,1)	–	(2 $\bar{1}$ $\bar{1}$ 2)	180	(2 $\bar{1}$ $\bar{1}$ 2)
(10 $\bar{1}$ 0)	(1,0,0)	–	(10 $\bar{1}$ 2) (11 $\bar{2}$ 1)	177	(10 $\bar{1}$ 1) (10 $\bar{1}$ 2) (11 $\bar{2}$ 1)

Notes: *T*—tension, *C*—compression.

According to the experimental results in Ref. [13], the initial stress needed to maintain the growth of the twins is smaller than the nucleation stress. And the initial stress is about 220 Mpa, which is closer to the computational results.

According to two different compression directions, (0001) and (10 $\bar{1}$ 0), the evolution process of deformation twins in pure titanium is also obtained in this article. The numerical results is shown in Figs. 3(a) and (b) and Table 2, and the corresponding experimental results cited from Ref. [14] is also shown in Figs. 3(a) and (b) and Table 2.

Fig. 3(a) and (b) and Table 2 indicate:

- When titanium single crystal was compressed along C-axis, computational results show that the (2 $\bar{1}$ $\bar{1}$ 2) and (10 $\bar{1}$ 0) twins would appear in titanium and (2 $\bar{1}$ $\bar{1}$ 2) twins is the primary type of twins (Fig. 3(a)), which is consistent with the experiment results obtained by Paton and Backofen [14].
- When titanium single crystal was compressed along (10 $\bar{1}$ 0) axis, computational results show that the (10 $\bar{1}$ 2) and (11 $\bar{2}$ 1) twins would appear in titanium (Fig. 3(b)), which is also consistent with the experiment results got by Paton and Backofen [14].

4. Conclusions

The evolution equations of the volume fractions of deformation twins are obtained by using the theory of inclusions and analyzing the Gibbs free energy of a system. The numerical results of the evolution equations (the critical twinning stress and the families of twins) are consistent with experimental results, which demonstrate the validity of the evolution equations in this article.

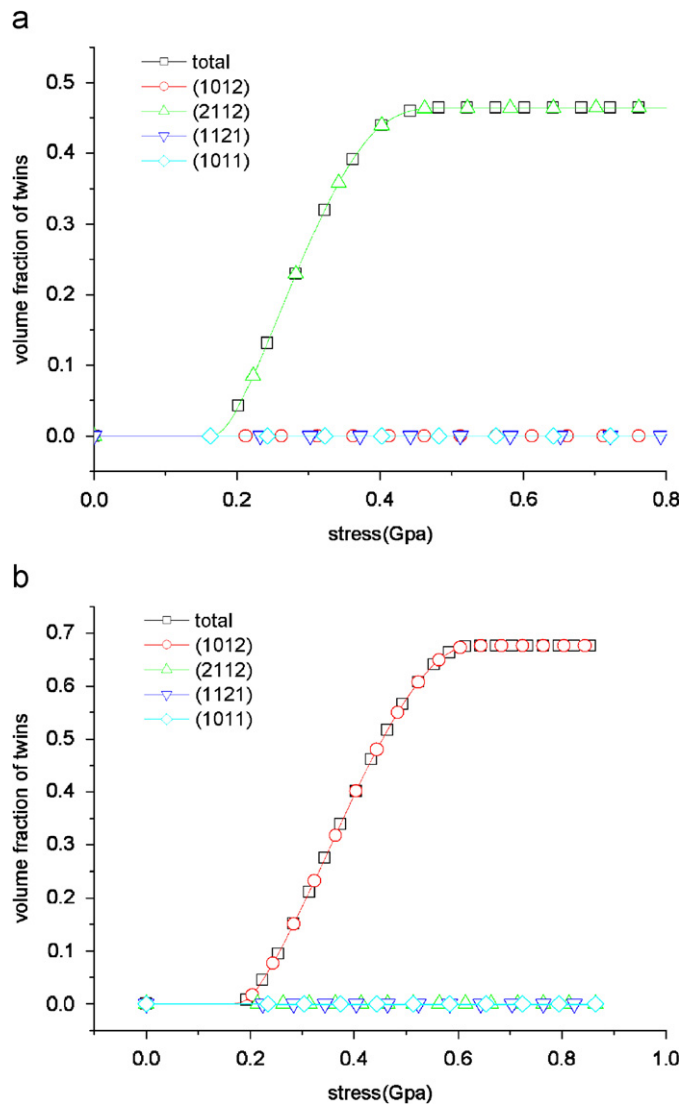


Fig. 3. Evolution of the volume fractions of deformation twins under compressive load at various directions. (a) C-axis; (b) (10 $\bar{1}$ 0) axis.

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