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Comparative Analysis of Stress Jumps in Metals and Intermetallic Compounds: II. Stress Macrojumps

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Abstract—Following the scheme proposed in part I of this study, analysis of two-stage straining in metals and intermetallic compounds is continued. Alternatives under which intermetallic compounds can experience stress macrojumps, i.e., abrupt increases or decreases in stress upon a change in temperature are discussed. The likely connection between the occurrence of a macrojump, corresponding to an abrupt decrease in stress, and the switching-on of a new slip system is explored. As a way of revealing stress macrojumps, two-stage straining experiments using specific temperature schemes and specific single crystal orientations are proposed.

INTRODUCTION

In part I of this study [1], we analyzed two-stage straining in fcc metals and intermetallic compounds. We identified the role that the transformations of dislocations to short- and long-lived barriers play in the deformation. The thermally activated formation of long-lived barriers in intermetallic compounds was found to govern the stress necessary to switch on dislocation sources and to determine its anomalous behavior with temperature (see equation (I.3.3)).[1] The condition for the onset of plastic flow at the second straining stage is given by equation (I.3.4). It implies the necessity for dislocation sources to start operating and for dislocations to overcome the elastic opposition presented by the microstructure produced at the first straining stage. We considered variants in which stress jumps in intermetallides are similar to those observed in metals and, just as in metals, are significantly less than the flow stress.

It was also noted in part I that intermetallic compounds can sometimes experience abnormally large stress jumps (see Fig. I.4 and [4, 8, 9] in part I). In part II, we make an attempt to explain the origin of such macrojumps and to see if it is possible for other types of macrojumps to occur.

1. STRESS MACROJUMPS IN TWO-STAGE STRAINING (WITHOUT A CHANGE IN THE SLIP SYSTEM)

A most distinct feature of the anomalous behavior of the yield stress with temperature is that the stress jumps $\Delta\sigma^{(T)}$ can be comparable in magnitude with the stress itself. Suppose that a TiAl specimen is subjected to two-stage straining at the same temperature as in [I.3], but the first stage takes place at a lower and the second, at a higher temperature, i.e., $T_1 < T_2$. Here, in contrast to metals, we may ignore the recovery of the dislocation structure (if the heating rate is high enough) because the microstructure created at the first stage is blocked owing to the $g \longrightarrow s'$ transformation of dislocations to barriers.

In the case at hand, the stresses that cause dislocation source to start operating (without a prestrain) are such that $\sigma_F^{(2)} > \sigma_F^{(1)}$, and the stress at the end of the first stage, σ_1, only slightly differs from $\sigma_F^{(1)}$. It then follows that $\sigma_F^{(2)} > \sigma_1$. Therefore, we at once find from (I.3.10) that at the second stage plastic flow commences at $\sigma_2 \approx \sigma_F^{(2)}$, that is, as if there were no prestrain.

By denoting the stress jump that occurs upon an increase in temperature as $\Delta\tilde{\sigma}^{(T)}$, we immediately find that $\Delta\tilde{\sigma}^{(T)} \approx \sigma_F^{(2)} - \sigma_F^{(1)}$. Here, we may neglect the contribution due to $g \rightleftharpoons s$ transformations, although, as is noted in [1], it is these transformations that determine the magnitude of $\Delta\sigma^{(T)}$. Thus, in this case, $\Delta\tilde{\sigma}^{(T)} \gg \Delta\sigma^{(T)}$. In other words, stress jumps display an asymmetry with respect to the change of sign of ΔT.

It is of interest to make experiments where one straining stage takes place at a very low temperature. According to Kawabata *et al.* [2], at below room temperature TiAl displays an abrupt increase in the yield stress. We will not discuss why this is so (see [I.6]). Schematically, the nonmonotone behavior of the function $\sigma_y(T)$ in TiAl is shown in Fig. 1 along with the intervals where the yield stress behaves differently with

[1] Here and elsewhere, the references to part I will be labeled with the Roman numeral I.

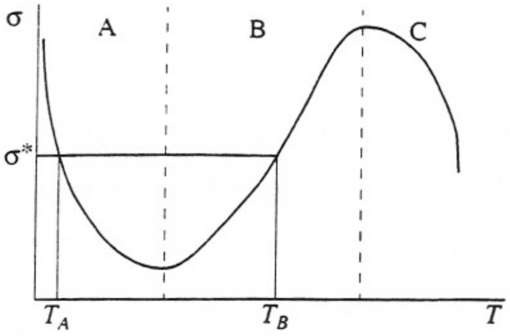

Fig. 1. Schematic representation of the nonmonotone behavior of the yield stress of TiAl with temperature.

temperature. Suppose that the specimen is subjected to two-stage straining at temperatures T_A and T_B, and that at each a stress σ^* is attained. Let us see what results can be expected in this case.

As before, we will use the C diagram shown in Fig. I.1 and equation (I.1.10) for $\sigma(T)$. Then, without a prestrain, the change of the dominant transformation with a rise in temperature will be described as

$$\sigma_s(T_A) \approx \sigma^*, \quad \sigma_{s'}(T_B) \approx \sigma^*. \tag{1.1}$$

Let the temperature vary from T_B to T_A. Then the blocked microstructure inherited from the first stage will contribute σ^* to $\sigma_2(T_A)$ defined by (I.1.7). To maintain the specified strain rate, an additional dislocation density $N_s(T_A)$ is needed. According to (I.1.6), it will, in turn, induce a strain $\sigma_s(T_A)$ defined by (I.1.8) and close to σ^*. As a result, we have $\sigma_2^2(T_A) \approx 2(\sigma^*)^2$. Thus, the stress at which plastic flow commences at the second stage is not σ^* (as would be the case without a prestrain), but a greater stress. Therefore, it seems legitimate to assert that a stress macrojump takes place in this case as well. It is easy to show that when the temperature changes from T_A to T_B, the stress jump will be significantly smaller; that is, $\Delta\tilde{\sigma}^{(T)} \ll \Delta\sigma^{(T)}$.

In the above cases, all the macrojumps take the same sign. To wit, a macrojump always implies an increase in stress, irrespective of whether the temperature is raised or lowered. The microstructure inherited from the first stage is blocked at the second stage and cannot provide for the specified amount of strain. If the fresh dislocations necessary for the purpose are difficult to inject into, a macrojump takes place.

2. TWO-STAGE STRAINING WITH A CHANGE OF THE SLIP SYSTEM

2.1. Does a New Slip System Go Operative and Why?

Although they were made to a different scheme, the experiments reported by Thornton *et al.* [I.10] help to clarify an issue common to any analysis of two-stage straining—the inheritance of the microstructure upon a change in temperature. In our opinion, the high value of σ_1 induced by cold deformation and preserved, as is noted in [I.10], upon a rise in temperature indicates that the microstructure does remain unchanged. That the yield stress ceases, in the circumstances, to behave anomalously with temperature can be readily explained using equation (I.3.10). To demonstrate, at temperatures such that $\sigma_F(T_2) < \sigma_1$ we immediately obtain from equation (I.3.10) that $\sigma_2 \approx \sigma_1$.

It is even more reasonable to expect that the microstructure will remain unchanged with a fall in temperature, when any risk of recovery is nonexistent. The results for TiAl (see Fig. I.3) likewise bear out that the microstructure is preserved. If we compare them with those for Ni_3Al (see Fig. I.4), we will face a paradox. On the one hand, the microstructure produced at the first stage keeps on opposing plastic flow in TiAl at the second stage. On the other, the microstructure is almost transparent to dislocations in Ni_3Al.

As will be recalled, the above microstructures consist of different types of dislocation. In Ni_3Al, they are solely $a\langle 101\rangle$ superdislocations. In TiAl, they additionally include $a/2\langle 110\rangle$ unit dislocations and $a/2\langle 112\rangle$ superdislocations. Every type has a blocking mechanism of its own [3, 4]. In what follows, we will not consider the $a/2\langle 112\rangle$ superdislocations because at below the temperatures of the yield stress peak they are seldom observed, if at all [4]. In the case of both $a\langle 101\rangle$ superdislocations and single dislocations, it is screw dislocations that are blocked so that the axes of the barriers run parallel to directions of the same type. Therefore, the findings of the subsequent analysis, undertaken primarily for Ni_3Al, may be applied to TiAl as well, but in no way automatically.

Consider the microstructure that emerges in Ni_3Al toward the end of the first, high-temperature stage owing to the action of one slip system. By virtue of the $g \longrightarrow s'$ transformations of screw superdislocations, this microstructure consists of identical Kear–Wilsdorf barriers parallel to the same $\langle 110\rangle$ direction. For brevity, we will refer to the blocked dislocation substructure as the framework, and to the axis of the barriers, as the framework axis. The barriers are indestructible within the region where $\sigma_y(T)$ shows an anomalous behavior, as noted previously. They can hardly be expected to go over into glissile superdislocations on cooling. Therefore, the framework is rigid and is inherited at the second, low-temperature stage of straining; that is, its density is preserved.

Let, at the second straining stage, the slip plane of a trial superdislocation be parallel to the framework axis. Then, the dislocation will have to overcome the elastic opposition presented by the framework because of (I.1.5). As a result, the stress $\sigma_2(T_2)$, at which plastic flow begins at the second stage, cannot, according to (I.3.4), fall below $\sigma_1(T_1)$.

The resistance that the framework presents to the trial superdislocation will, however, be different if its slip plane is not parallel to the framework axis. No segments parallel to the trial dislocation can arise on the dislocations that constitute the framework because it is rigid. As a result, the framework will present almost no elastic resistance to the trial dislocation. This is where, as we think [I.12], [5], lies the possibility for a sharp decrease of stress, that is, for a stress macrojump, to occur on passing to the second stage.

For this possibility to become a reality, the stress required to initiate dislocation sources, $\sigma_F(T)$, should decrease with decreasing temperature; that is, it should exhibit an anomalous temperature dependence. A change to a new slip system can, however, cause a decrease in the Schmid factor, and this can, in turn, make up for the decrease in stress. Therefore, for the new slip system with a Schmid factor f_2 to be able to assure a certain observed value of $q = \sigma_1/\sigma_2$, a necessary condition is

$$q\frac{\sigma_y(T_2)}{\sigma_y(T_1)} < \frac{f_2}{f_1} < 1, \tag{2.1}$$

where $\sigma_y(T_1)$ and $\sigma_y(T_2)$ are the yield stresses (at the corresponding temperatures) without prestrain, and f_1 is the Schmid factor of the slip system operative at the first stage.

The question as to why a new slip system with a smaller Schmid factor goes operative at the second stage implies the question as to why it does not go operative at the first stage. Using (I.3.3), we immediately find that for the slip systems in question the difference between their initiating stresses is proportional to $\exp\left(-\frac{U^F_{gs'}}{kT}\right)$. This signifies that for a slip system with a smaller Schmid factor it is more difficult to go operative at a higher than at a lower temperature. This is important because otherwise this slip system would create a framework of its own and would not be able to support a stress macrojump.

This prompts one more question: Are the dislocation sources of the primary slip system operative at the second stage? The views set forth in [1] do not rule this out, but flow does not happen in the primary system because the stress is smaller than $\sigma_1(T_1)$.

Hence, the following dilemma presents itself: Either the primary slip system remains operative at the second stage and the stress required is not smaller than $\sigma_1(T_1)$, or a new slip system goes operative, which has a smaller Schmid factor but meets almost no elastic opposition from the framework. The results of experiments with Ni_3Al and TiAl offer a wide choice of options.

Even if the change to the second stage is accompanied by a decrease in the stress, the framework will still manifest itself, but in a different role. The rigid framework acts as a "forest" for dislocations in the new slip system. The contribution σ_f to $\Delta\sigma$ associated with the intersection of the forest (see (I.1.13)) can be considerable owing to the high density of the framework dislocations.

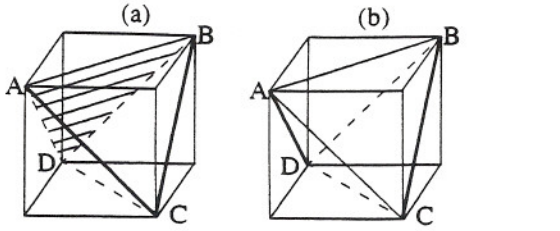

Fig. 2. Various relative positions of the framework axes: (a) framework axes **CA** and **CB** are parallel to the same octahedral plane; (b) framework axes **CB** and **AD** are parallel to the same cubic plane.

2.2. The Search for a New Slip System

At first glance, this section and the next may seem irrelevant. However, apart from adding more detail to the rather general approach set forth above, they contain specific proposals that can help one to interpret the complicated and contradictory experimental findings. We will try to identify first the type of microstructure inherited from the first stage that makes a new slip system go operative at the second stage, and then the orientations of the strain axis that make it possible.

When operation of the primary slip system results in the formation of a framework, its axes run, as already noted, parallel to the same $\langle 110\rangle$ direction and thus belong to two octahedron planes at the same time. Two other $\{111\}$ planes are possible slip planes for the new system. Therefore, if, at the end of the first straining stage, this microstructure is observed, the new slip system is generally very simple to identify. It is the system whose slip plane is intersected by the framework axes and whose Schmid factor is the largest possible in that plane.

If, on the other hand, two slip systems differing in the Burgers vector are operative at the first stage, two possibilities are equally likely, namely, either the double-framework axes parallel to these vectors will belong to the same octahedral plane or to the same cubic plane, being mutually perpendicular in the latter case (see Fig. 2).

If the first possibility is true, there remains only one $\{111\}$ plane intersected by both axes of the framework. With respect to the dislocations gliding in that plane, the framework acts as a forest. Suppose that we observe a framework with its axes parallel to **CA** and **CB** (see Fig. 2a). Then, in Thompson's notation, the plane (c), shown shaded in Fig. 2a, is the only $\{111\}$ plane that does not contain any framework axes. The micrograph in Fig. 3 shows the dislocation structure observed [I.4] in Ni_3Al. It exhibits screw dislocations lying in the same $\{111\}$ plane and blocked along two $\langle 110\rangle$ direc-

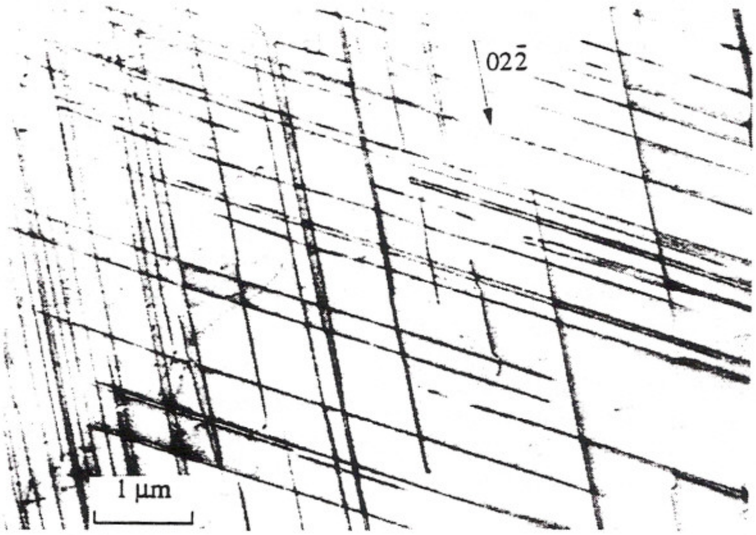

Fig. 3. Transmission electron micrographs of the dislocation structure in Ni_3Al deformed first at 875 K and then at 300 K. A bright-field image of long screw dislocations in a primary (111) plane.

tions. This is an example of the case we have just discussed. Therefore, the observed stress macrojump occurs, as we think, because a new system with a slip plane intersected by the axes of the blocked dislocations becomes operative.

In the second case, on the contrary, there remains not a single $\{111\}$ plane that would not contain double-framework axes (see Fig. 2b). A search for a new slip system can hardly be successful in such a case: dislocations of any slip system meet the elastic opposition of the framework. It is even less likely to expect the occurrence of a stress macrojump when an even greater number of slip systems are operative at the first stage. Presumably, this is the case that occurred in the experiments of Thornton *et al.* [I.10], when the prestrain was rather heavy.

2.3. Symmetry Analysis of Uniaxial Deformation

It is symmetry analysis that has proved most efficient in finding out what orientations the deformation axis should have in order for a particular type of microstructure to be produced. Here, we will give a brief account of the main findings. We regard uniaxial deformation as an external influence and use the known principle of symmetry superposition. According to it, application of an external influence preserves only those symmetry elements that are common to the crystal and the external influence [6].

Hence, for the $L1_2$ and $L1_0$ superstructures we immediately find that mutually perpendicular directions of the $\langle 101\rangle$ type will remain crystallographically equivalent under uniaxial deformation only if the **t** axis, being an axis of deformation, lies in a cube plane. Then it may be expected that the Burgers vectors of two primary slip systems having the same Schmid factor and, accordingly, the axes of the double framework they form, will run parallel to these $\langle 101\rangle$ directions. Such a framework consists of superdislocations in the case of Ni_3Al and of either superdislocations or single dislocations in the case of TiAl. In either case, however, it will inhibit the occurrence of a stress macrojump. Therefore, it is difficult to expect, in particular, a stress macrojump when the orientation is such that the **t** axis runs parallel to an edge of the cube or to a diagonal of its face.

When TiAl is subjected to two-stage straining [I.3], the direction of the **t** axis is close to [010]. No stress macrojump is observed in this case (see Fig. I.3). As follows from the foregoing, this can happen not only with an exact [010] orientation, but also when the **t** axis deviates into the cube plane.

Going back to the experiment with Ni_3Al [I.4], where the orientation is likewise close to $\langle 001\rangle$, we conclude that the observed microstructure (see Fig. 3) could not arise with an exact $\langle 001\rangle$ orientation. This could, however, happen if the **t** axis deviated into a plane of the $\{110\}$ type. This can be proved as follows. Using again the principle of symmetry superposition, we can show that in the $L1_2$ superstructure for an arbitrary **t** axis lying in some $\{110\}$ plane, two $\langle 101\rangle$ directions that belong to the same octahedral plane and are a mirror image of each other in the $\{110\}$ plane will remain crystallographically equivalent even under uniaxial deformation. For example, if we wish, in the case of the orientation close to [001], to have a double framework with axes **CA** and **CB** (see Fig. 2a), the **t** axis must deviate into the $(1\bar{1}0)$ plane. In this case, the double-framework axes will belong to the same

(111) plane, and a macrojump will be possible (see the previous section).

Symmetry analysis reveals only an idealized representation of how slip systems with crystallographically equivalent directions of Burgers vectors and identical Schmid factors go operative. The actual picture is far more complicated. Nevertheless, it does give insight into some tendencies in the formation of a particular type of framework upon various orientations.

Lastly, consider two-stage straining in Ni_3Al for two most commonly used orientations, [111] and $[\bar{1}32]$.

Let the **t** axis be parallel to [111] so that the maximum Schmid factor corresponds to the Burgers vectors **DA**, **DB**, and **DC**, and that it is zero for all others. If the first stage terminates in forming a framework with axes parallel to the above vectors, the only slip plane that does not contain framework axes will be the (*d*) plane. Because in that plane any of the Schmid factors is zero, it is not possible for a new slip system to become operative and for a stress macrojump to occur. Suppose that the **t** axis deviates from the [111] direction in, say, the $(11\bar{2})$ plane so that only one slip system, **DC**(*a*), has a maximum Schmid factor. Then, at the second straining stage the likely slip plane will be the (*c*) plane, where high Schmid factors correspond to the vectors **DA** and **DB**, from which the Burgers vector of the new system is chosen. As a result, a stress macrojump may be expected to occur.

Let now the **t** axis be parallel to $[\bar{1}32]$. Then the slip system operative at the first straining stage will be **BA**(*d*), for which the Schmid factor f_1 is maximum and equal to 0.467. This will result in a framework with the **BA** axis. The likely slip planes at the second stage, i.e., (*b*) and (*a*), do not contain framework axes. In these planes, the largest Schmid factor is associated with the **CD**(*b*) system, for which $f_2 = 0.348$. From the $\sigma_y(T)$ curve given in [7], we obtain $\sigma_y(T_1)/\sigma_y(T_2) \approx 5$. Then, as follows from (2.1), the stress will decrease such that $\sigma_1/\sigma_2 \cong 3.75$ if a new slip system with this Schmid factor f_2 becomes operative at the second straining stage.

The effect under consideration, consisting of a strong decrease in the stress with decreasing straining temperature, is unusual. It is not surprising, therefore, that searching the factor responsible for the effect turns into a detective investigation. At least two questions should be clarified in this case above all. First, is there a connection between the microstructure of a preliminary deformed alloy and the occurrence of the effect, i.e., what is the structure of the dislocation framework that makes it possible to observe the effect and what is the structure that prevents doing this? Second, what are the conditions that favor the formation of this or that structure of the framework?

As was shown above, if the framework has a simple, regular structure, this favors the occurrence of a stress macrojump. A complicated structure may cause the effect to vanish. This may take place either when the preliminary deformation is large [I.10] or dislocations of several types are present in the structure, as may be the case in TiAl [I.3].

The effect may vanish, as it follows from the above analysis, if a "cross"-type framework arises, e.g., as a result of two slip systems with mutually perpendicular Burgers vectors being operative simultaneously. How can such a structure be obtained? It may seem that it can appear if the deformation axis lies, as was said above, in a {100} plane. However, the simultaneous initiation of the two above-mentioned slip systems may be difficult for reasons that are still unclear. This may take place, for example, if one of the operative slip systems is initiated (e.g., because of a departure from an exact orientation) earlier than the other and goes ahead, as strain increases, because of an avalanchelike nature of the dislocation multiplication process.

Now, we may try to construct a framework with a cross-type structure by introducing one more high-temperature strain stage. We will use orientations at which the Schmid factor in one of the slip systems is much greater than in the other slip systems. Let the first straining stage (at a temperature of T_1) be carried out at the $[\bar{1}32]$ orientation. By the end of the first stage, as was said above, there would form a framework of blocked screw dislocations with axes parallel to **BA**. The additional straining stage, following cooling, again will be conducted at T_1, but using another deformation axis, though of the same type as in the first stage.

We may chose a deformation axis that ensures the Schmid factor is greatest for a system with Burgers vector perpendicular to **BA**. This may be, e.g., the [132] orientation, for which the Schmid factor is largest for the **CD**(*b*) system. We may expect that precisely this system will be switched on at the additional stage of deformation. As a result, by the end of this stage, a dislocation framework with a structure of cross type may form. We believe that a transition to the low-temperature straining stage would not be accompanied by a stress macrojump if the [132] orientation is used.

We may select the deformation axis for the additional stage in a different way, namely, in such a manner that that slip system would be initiated in which both the Burgers vector and **BA**, in contrast to the previous case, are parallel to the same {111} plane. This may be the $[\bar{1}23]$ orientation, at which the **BC**(*d*) system will be operative. The structure of the resultant framework in this case will enable observing stress macrojumps upon decreasing temperature.

CONCLUSION

Using a unified approach, we attempted to analyze stress jumps that may occur upon temperature changes in fcc metals and intermetallic compounds exhibiting an anomalous temperature behavior of yield stress. We investigated the role that short- and long-lived barriers play in the course of plastic deformation both at fixed and varying temperatures. Some light is thrown on how the thermally activated blocking of dislocations, affects the initiation of dislocation sources and the shape of the stress–strain curve upon two-stage straining in intermetallic compounds. The analysis is based on a concept according to which the stress necessary for plastic flow to commence at the second straining stage is related by equation (I.3.4) to the stress governing the elastic opposition presented by the frame inherited from the first stage and to the stress necessary for dislocation sources to become operative at the second stage.

We examined conditions under which a significant change (a rise or a fall) of stress, that is, a stress macrojump, can occur in intermetallic compounds as the first straining stage gives way to the second. To check if the concept of a relation between the dislocation-framework structure and the possibility to observe stress macrojumps is valid, we suggest new experiments on two-stage deformation, which should be performed with an appropriate choice of temperatures and orientations.

The further development of the suggested approach to the description of plastic deformation, including stress jumps, should involve the following. The equation of detailed balance should be supplemented with an equation describing the multiplication of dislocations. This equation may be written in a form similar to that used to describe the evolution of a population in biology. At the same time, it is essential to take into account the fact that the stress levels governing both the initiation of dislocation sources and the onset of plastic flow are of smeared rather than sharp character. Therefore, equations (I.1.3), (I.1.5), and (I.3.1) should be extended to include factors allowing for this "smearing". Such a modification of the overall scheme makes it possible to describe the transition region between elastic and plastic deformation (in particular, a nonmonotone dependence of $\sigma(\varepsilon)$) observed sometimes upon both single- and double-stage straining.

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