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Dislocation-Obstacle Interactions and Mechanical Properties of Intermetallics

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Abstract. The mechanical properties of materials are discussed for different configurations of the obstacles (in series or in parallel), different dislocation-obstacle regimes (exhaustion or crossing) and different obstacle strengths (one type of obstacle or a spectrum of obstacles of different strengths). The models proposed for Ni₃Al are compared in what concerns the yield stress anomaly and the partial reversibility of the flow stress upon a decrease of the temperature.

1. INTRODUCTION

The mechanical properties of materials can in theory be explained in terms of several microscopic processes including interactions between dislocations and obstacles. In particular, this holds true for intermetallic alloys which exhibit a remarkable variety of unusual mechanical properties and dislocation mechanisms.

Determining the nature of the obstacles opposing to dislocation movements is the first step of microscopic studies. Reliable models of mechanical properties can however be set up only when the exact roles of dislocation-obstacle interactions are known at a microscopic scale including a large number of dislocations and obstacles. This article is thus aimed to discuss in a very simple way the relation between several types of dislocation-obstacle interactions and some mechanical properties of intermetallic alloys.

2. THE ELASTIC LIMIT

The plastic deformation of materials due to the motion of dislocations is described by the Orowan law: $\dot{\epsilon} = \rho b v$, where $\dot{\epsilon}$ is the strain rate, ρ is the density of mobile dislocations, b is their Burgers vector, and v is their average velocity. In constant strain-rate tests, the stress may adjust itself so as to maintain either a constant value of v , or a constant value of ρ . These two situations correspond to

pure obstacle crossing and pure exhaustion mechanisms, respectively. These two mechanisms are described for several types of obstacles in what follows.

2-1 Single type of obstacle

When a crystal containing only one type of obstacle is strained, the mobile dislocations are progressively locked against the obstacles. In order to allow for further deformation, new mobile dislocations are nucleated which are also locked progressively at the obstacles, and so on. This process leads to a rapid increase in the flow stress for two reasons :

- the internal stress due to the accumulation of locked dislocations increases,
- the sources of mobile dislocations are progressively exhausted, and the different processes leading to the activation of new mobile dislocations need a higher stress. This may correspond to the activation of new sources on shorter segments.

The importance of these two contributions is discussed for Ni_3Al in §3-2-2 and §4.

When the stress increases to the critical value σ_{obst} which allows for obstacle crossing, the exhaustion process stops, the strain hardening rate decreases and the deformation goes on without any additional dislocation multiplication.

When the exhaustion stage is short, the yield stress (namely the flow stress for $\epsilon = \epsilon_{\text{el}}$) can be identified with the stress necessary to cross through the obstacles. The deformation is then controlled by a crossing process, and the corresponding stress-strain curve is described schematically in fig. 1a. When the exhaustion stage is long, however, the stress-strain curve is like in fig. 1b and the deformation is controlled by an exhaustion process up to high strains. Accordingly, the yield stress is more difficult to define, and the strain-hardening coefficient at yield is higher than in the first case.

When the applied strain rate $\dot{\epsilon} = \rho b v$ is increased, the stress increases so as to increase ρ and v .

Fig. 1 : Schematic description of stress-strain curves, for one type of obstacle (σ_{obst}) or several types of obstacles in parallel (σ_{min}) and a) a crossing mechanism, b) an exhaustion mechanism.

The stress-strain rate dependence can be described by the apparent activation area, $A_{ap} = \frac{kT}{b} \frac{\partial \ln \dot{\epsilon}}{\partial \sigma}$,

where σ is the applied stress. It can be expressed as :

$A_{ap} = \frac{kT}{b} \left(\frac{\partial \ln v}{\partial \sigma} + \frac{\partial \ln \rho}{\partial \sigma} \right) = A + \frac{kT}{b} \frac{\partial \ln \rho}{\partial \sigma}$, where A is the activation area describing the movement of individual dislocations. When the deformation is controlled by a crossing process, A can be small if the crossing process is strongly thermally activated. The second term is however difficult to estimate (experiments in magnesium showed that it can be substantially larger than the first [1]). When the deformation is controlled by an exhaustion mechanism, A can be determined by interactions with weak obstacles.

2.2 Obstacles of different strengths

In most real cases, dislocations interact with a spectrum of obstacles of different strengths ranging between $\sigma_{\min}$ and $\sigma_{\max}$. Different behaviours are then observed according to whether the obstacles are acting in parallel or in series.

When the obstacles are acting in parallel, the stress increases to $\sigma_{\min}$ for which the weakest obstacles are crossed. Then, the dislocations are able to move over long distances. The situation is thus the same as in the above case, with σ_{obst} being replaced by $\sigma_{\min}$. In particular, the two regimes - exhaustion and crossing processes - are still well defined.

When the obstacles are acting in series, however, the situation is slightly more complex. The flow stress increases first to $\sigma_{\min}$ which allows for crossing the weakest obstacles and decreasing the strain-hardening rate. Dislocations are however still locked against the strongest obstacles, in such a way that exhaustion is still important. Exhaustion decreases to zero only at $\sigma_{\max}$. Accordingly, the stress-strain curve is thought to be more rounded than in the case of obstacles in parallel, and the exhaustion regime may extend over a larger strain range (fig. 2). The deformation at yield is thus

Fig. 2 : Schematical description of a stress strain curve, for several types of obstacles acting in series (exhaustion mechanism).

likely to be controlled by the exhaustion regime in this case. For a stress ranging between $\sigma_{\min}$ and $\sigma_{\max}$, crossing and exhaustion processes thus take place simultaneously. As in § 2-1 above, changing the applied strain rate is accommodated by a change in both the density and the velocity of mobile dislocations. Since mobile dislocations are interacting with obstacles of strength $\sigma_{\min}$ to σ (where σ is the flow stress), and, provided the crossing processes are thermally activated, the activation area A corresponds to these obstacles. The second term corresponding to the change in mobile dislocation density with stress is again difficult to estimate.

3. YIELD-STRESS ANOMALIES

Many intermetallic alloys exhibit an anomalous increase of the yield stress with increasing temperature (yield stress anomaly) in their intermediate temperature range. This unusual behaviour has to be taken into account in the design of new materials with attractive mechanical properties at high temperatures and good resistance to brittleness at low temperatures. Generally speaking, the plastic properties of materials with a normal stress-temperature dependence are such that high yield stresses at high temperatures are coupled with such high yield stresses at low temperatures that little plastic deformation is allowed and brittle fracture occurs. On the contrary, materials with an anomalous stress-temperature dependence can deform under low stresses at low temperature, which may contribute in some cases to increase the plastic relaxation at crack tips and reduce the brittleness.

3.1 Possible origins of yield-stress anomalies

When yield stresses are controlled by an exhaustion mechanism, yield stress anomalies can arise from a more rapid dislocation locking, namely an increase of the obstacle density with increasing temperature (fig. 3a). Increasing both the density and the strength of the obstacles is however more efficient in obtaining a yield stress anomaly (fig. 3b).

When deformation is controlled by a crossing process, yield stress anomalies may arise from an increase in the obstacle density with increasing temperature. This yields the same result as increasing the strain rate in the same proportion when the obstacle density is kept constant. This effect can be important when the crossing mechanism is strongly thermally activated. It must however be large enough to overcome the normal effect of temperature on the crossing mechanism which is also necessarily large for the same reason. Accordingly, yield stress anomalies are more likely to originate from an increase in the strength of the obstacles with increasing temperature (fig.4). If the obstacles are localized or discontinuous along dislocations (fig. 5a), they can be by-passed by mobile

Fig. 3 : Possible origins of yield stress anomalies, for several types of obstacles in parallel ($\sigma_{\min}$) or in series ($\sigma_{\max}$), and an exhaustion mechanism. a) Increase in the density of obstacles. b) Increase in the density and the strength of the obstacles.

Fig. 4 : Origin of the yield stress anomaly for several types of obstacles in parallel ($\sigma_{\min}$) or in series ($\sigma_{\max}$) and a crossing mechanism.

Fig. 5 : Different possible topologies of dislocation-obstacle interactions : a) by passing and cutting, b) cutting (intrinsic unlocking)

dislocation segments bowing in the free areas. In this situation where obstacles are acting in parallel, their strength can be increased either by increasing their height or by decreasing their separation, the second situation being more often considered. On the contrary, if the obstacles constitute a continuous front opposing dislocation movements (fig. 5b), they are necessarily cut (intrinsic unlocking). In this case where obstacles are acting in series, yield stress anomalies can only arise from an increase in their height with increasing temperature.

3.2 Principles of the different proposed models

Details on the models which have been proposed to explain yield stress anomalies in different intermetallics can be found elsewhere [2-6]. Only the principles of these models are discussed here, and tentatively classified according to the above remarks.

3.2.1 Dynamic strain ageing

In L_{12} stabilized Al_3Ti , the weak yield-stress anomaly between 300°C and 500-700°C [7-8] is clearly related to strain instabilities such as the Portevin-Le Chatelier effect, and to a negative value of the stress-strain rate sensitivity [8]. Microscopic observations reveal no dissociation and no directionality of $\langle 110 \rangle$ superdislocations in this temperature range. Accordingly, the weak yield stress anomaly has been attributed to dynamic strain ageing effects, namely to an increase in the dislocation-solute atoms interaction with increasing temperature.

3.2.2 Formation of Kear-Wilks locks

In Ni_3Al in octahedral slip, many studies which have been reviewed in [2-5] have led to several common conclusions, but also to several different interpretations. It is now accepted that the obstacles against dislocation movements are due to the cross slip of screw superdislocations into cube planes. When dislocations glide in octahedral planes, they are dissociated into two superpartials separated by an antiphase boundary (APB) ribbon. Due to a lower APB energy in the cube plane and to a torque force associated with elastic anisotropy [9], the leading superpartials tend to cross-slip and glide over various distances in the intersecting cube plane. When the glide distance is large, this process leads to the formation of complete Kear-Wilks locks. When the glide distance is smaller than the

dissociation width of superdislocations, this process leads to the formation of incomplete Kear-Wilks locks which are dissociated partly in the octahedral plane, partly in the cube plane. In both cases, however, the screw superdislocations are locked. The stress for unlocking incomplete and complete Kear-Wilks locks by another cross-slip process into the octahedral plane has been computed recently [10-11]. It increases with increasing glide distance in the cube plane. The models proposed are however different in the topology and the exact role of the obstacles.

In the local pinning model [12-13], glissile screw superdislocations tend to cross-slip locally into the cube plane. The velocity of dislocations is however assumed to be high enough to prevent from the extension of locking along the whole dislocation. In such conditions, mobile dislocations can break away dynamically from the local pinning points. Only one type of obstacles are acting in parallel, and they are by-passed by the glissile segments. Accordingly, the flow stress is directly related to the density of pinning points along dislocations, and the yield stress anomaly results from a decrease in their separation.

The kink model has similar properties, although it is based on different assumptions [14-16]. In this case, screw superdislocations are assumed to be locked along their whole length. Observations however show that such dislocations also exhibit macrokinks which are short non screw segments connecting two long screw segments. If these macrokinks can act as sources, they can nucleate new glissile dislocations which subsequently annihilate with the adjacent locked screw segments. Accordingly, a large spectrum of obstacles are acting in parallel (if superdislocations exhibit several adjacent screw parts) and they can be by-passed at the macrokinks. Since the operation of sources at macrokinks is easier when the height of the kinks is larger, the increase in strength can be interpreted by a decrease in the average kink height with increasing temperature.

The double cross-slip model [17-19] is also based on the existence of long locked screw superdislocations, connected by macrokinks. Since in situ observations show that macrokinks are very mobile along screw dislocations, it is however assumed that they cannot act as dislocation sources. With this hypothesis, by-passing cannot take place, and locked dislocations can go on gliding over long distances only by series of double octahedral-cube-octahedral cross slip processes (obstacles opposing a continuous front to dislocation movement, acting in series). Since the obstacles can be incomplete Kear-Wilks locks with various strengths, the stress-strain curve is however expected to be as in fig. 2, namely the flow-stress is thought to be controlled by an exhaustion process below $\sigma_{\min}$, a mixture of exhaustion and intrinsic unlocking processes between $\sigma_{\min}$ and $\sigma_{\max}$, and an intrinsic unlocking process alone at $\sigma_{\max}$. Accordingly, the yield-stress anomaly results from a more rapid exhaustion below $\sigma_{\max}$, with increasing temperature. The temperature dependent exhaustion mechanism is described in [19]. An increase of the obstacle strength may also contribute to increasing the yield stress, at increasing temperature, as described schematically in fig. 3b. Such an increase in the obstacle strength with increasing temperature may result from diffusion processes as in the case of Al_3Ti [18, 19]. Since the total dislocation density does not increase substantially

with increasing temperature, at constant strain, it can be concluded that hardening does not result from internal stresses only. The exhaustion of sources is thus likely to be important, at least in this case.

The two first models are based on a by-passing mechanism, whereas the third is based on a cutting (intrinsic unlocking) mechanism. Whenever dislocations are liable to take alternately glissile and sessile configurations, intrinsic unlocking and by-passing are competing mechanisms. These two possibilities are illustrated schematically in fig. 6, for two situations which correspond respectively to the initiation (fig. 6 a-d) and the extension (fig. 6 e-h) of the locking process. In both cases, glissile dislocations have a high velocity V . It is also necessary to take into account the velocity V' of the transition from glissile to sessile configurations along the direction of the sessile configuration (the screw direction in this case). The driving force for this movement may indeed be high, since it leads to a substantial decrease of core energy due to cross slip into the cube plane. Now, two situations can arise according to whether $V' \gg V$ or $V' \ll V$.

By passing can occur only if $V' \ll V$. The two starting configurations (fig. 6 a and e) then lead respectively to the basic hypotheses of the local pinning and kink models (fig. 6 c and g) (this illustrates that these two types of model are in fact very similar to each other). If, on the contrary, $V' \gg V$, locking extends over the whole dislocation (fig. 6 b and f), and as a result subsequent unlocking is necessarily initiated intrinsically (fig. 6 d and h). It is worth noting that the recent computations of Mills and Chrzan [16] lead only to the by-passing mechanism because the mobility of the constriction is not taken into account (corresponding to $V' = 0$). In fact, the result depends on the frictional force acting on the glissile-sessile transition point. In Hirsch's model [15], the condition $V' \ll V$ is met because pinning points limit the extension of locking during the glide process.

3.2.3 Other situations

In many other situations which have been analysed in [2], dislocations are subjected to high Peierls-type stresses in the temperature domain of yield-stress anomaly, but cross-slip processes similar to those observed in Ni_3Al are either impossible or unlikely. The last condition is obviously met for ordinary dislocations in TiAl . In this case, in situ experiments should be used in order to determine the exact role of pinning points with respect to Peierls forces, and the exact role of exhaustion with respect to crossing. A model of yield stress anomaly can indeed be set up only when the mechanisms controlling deformation at yield are well known.

4. EFFECT OF A HIGH TEMPERATURE PREDEFORMATION IN Ni_3Al

Amongst the anomalous mechanical properties of Ni_3Al , the most difficult to explain is probably the reversibility of the flow stress upon a temperature decrease. When a sample is predeformed at high temperature in the domain of yield stress anomaly, and subsequently deformed at a lower

Fig. 6 : Conditions for observing by-passing and intrinsic unlocking mechanisms (from [20]).

temperature, the second stress-strain curve is approximately that of a virgin sample, except for a higher stress due to high temperature strain-hardening.

In all the models discussed in §3 above, the obstacles are nucleated on moving dislocations, with the help of thermal activation, and destroyed when they are cut or by passed. When the temperature is decreased, the new obstacles which are formed during the glide process are thus less efficient, and a decrease in the flow stress is expected on condition that a sufficiently high density of mobile dislocations are present in the crystal at the onset of the second deformation test. This condition is not met in all cases, as discussed below.

If the flow stress is controlled by a crossing mechanism, and if obstacles are acting in parallel (fig. 7a), all dislocations are in front of obstacles of strength $\sigma_{\min 2}$ to $\sigma_{\max 2}$ after the predeformation. Since dislocation sources with critical stress lower than $\sigma_{\min 2}$ are probably exhausted, some dislocations must unlock at the onset of the low temperature deformation (except if sources are regenerated upon unloading, as assumed by Ezz and Hirsch [21]). Accordingly, the flow stress must increase to $\sigma_{\min 2}$ before decreasing to $\sigma_{\min 1}$.

If the obstacles are acting in series, the stress is $\sigma_{\max 2}$ during the predeformation test, and mobile dislocations glide easily across obstacles of strength $\sigma_{\min 2}$ to $\sigma_{\max 2}$. If the crossing mechanisms are highly thermally activated, they need however non zero (although very short) waiting times. A substantial density of mobile dislocations are thus in front of obstacles $\sigma_{\min 2}$ to $\sigma_{\max 1}$, at the beginning of the second deformation test. If the density of dislocations at obstacles $\sigma_{\min 2}$ to $\sigma_{\max 1}$ is high enough to ensure plastic deformation at $\sigma_{\max 1}$, there is no transient as described schematically in fig. 7b.

Fig. 7 : Reversibility of flow-stress upon a temperature decrease, for a crossing mechanism (schematic description)

a) Obstacles in parallel, b) Obstacles in series.

Similar results are obtained in the case of exhaustion mechanisms, provided the exhaustion of sources contributes substantially to strain hardening, as described schematically in fig. 8. In the case of obstacles in parallel, the stress must increase to σ before decreasing to $\sigma_{\min 1}$, in order to create new mobile dislocations (fig. 8a). In the case of obstacles in series, however, dislocations in front of obstacles of strength $\sigma_{\min 2}$ to $\sigma_{\max 1}$ can subsequently glide under the stress $\sigma_{\max 1}$ (fig. 8b).

Conversely, the stress cannot decrease upon decreasing the temperature if the strain hardening results only from the internal stress field of locked dislocations, unless intensive recovery takes place.

Fig. 8 : Same as fig. 7, for an exhaustion mechanism (when hardening results from the exhaustion of sources).

a) Obstacles in parallel. b) Obstacles in series.

The local pinning model and the kink model may correspond to fig. 7a. In the local pinning model, deformation is however due to a low density of mobile dislocations gliding at a high speed. When the deformation test is stopped, the mobile dislocations are transformed into long Kear-Wilsdorf locks which cannot move further. When the sample is strained again, the few mobile dislocations which ensure plastic deformation are assumed to be nucleated easily. Accordingly, there is no need to reach the stress σ_{min2} when the deformation temperature is decreased, which can explain the experimental observations.

Conversely, the decrease in flow stress cannot be explained easily in the kink model since the behaviour described in fig. 7a may be observed (except if sources are regenerated upon unloading, as assumed by Ezz and Hirsch [21]).

Lastly, the double cross-slip model corresponds to fig. 8b. It can thus explain the experimental results.

5. CONCLUSION

This short review of the different types of dislocation-obstacle interactions shows that several situations can arise, according to whether a single type of obstacle, or a spectrum of obstacles of different strengths, are acting in series or in parallel. Even if the obstacles are well determined (e. g. Kear-Wilsdorf locks in Ni_3Al), these different situations lead to quite different mechanical properties.

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