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Climb model of dislocations in oxides

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Starting with a phenomenological hypothesis, a non-stoichiometric climb model of dislocations in oxides is suggested. Such a model is based on the different behaviours of the oxide components and may be summarized in the following way. A gliding dislocation is stopped by an obstacle. The faster ions diffuse either to or along the dislocation and aggregate to form coherent clusters in the lower part of the extra-half planes. These clusters may convert into more stable forms, such as dislocation loops, when they reach a certain size. The initial dislocation and the dislocation loop react and lead to a climb mechanism. Under the action of stress the pinning dislocation could then glide again and leave behind "interstitial loops". Such a climb model is compared to the classical stoichiometric one and developed through the example of a binary oxide. Extension to more complicated material involving "ionic molecule" aggregation is suggested.

1. Introduction

Experimental data concerning the plasticity of oxides, often exhibit considerable discrepancies even for the same material. It is, therefore, quite difficult to identify the fundamental mechanism controlling the plastic deformation behaviour. In general, the problem is dealt with by making a parallel study between experimental results and relatively simple models deduced from studies carried out on metals. Such is the case for dislocation climb in oxides. In fact, in oxides, (or in ionic crystals in general) little attention has been paid to the simple fact that there is often very different behaviour for the two sublattices and that subsequent defect mobilities are often quite different.

A direct comparison between climb of the dislocations in oxides and in pure metal is, therefore, no longer obvious. Nevertheless, a useful parallel with metallic solid solutions may be convenient for the definition of an effective diffusion coefficient. Fortunately, experimental data may be clarified when one of the ionic species does diffuse faster than the other.

On the basis of a classical climb model of the dislocation, the climb process is considered as being controlled by the displacement of the slower component of the oxide. A comparison with other experiments such as radio-tracer diffusion, is then possible. When the agreement is good the fundamental mechanism controlling the plasticity is thought to be found. Otherwise, either such complementary mechanisms as, for instance, jog formation, are added to the classical climb process, or else completely different rate-controlling mechanisms are considered. Thus, the classical concept of climb of dislocations in metals is applied to the oxides. However, taking into account the composition of the extra-half planes of the dislocations, climb is supposed to arise from absorption or emission of point defects on each of the sublattices in stoichiometric proportion. This process is rate-limited by the displacement of the slower ion. Otherwise, an effective diffusion coefficient may be considered.

The complexity of the oxide dislocation core, particularly when there are very large numbers of atoms per unit cell, the quite different behaviour of the two sublattices, the large point defect concentration which may be present in the matrix, due to the high temperature of the experiment and/or a greater or smaller deviation from the stoichiometry, may lead to a difference in opinion from such a classical picture. From recent experiments of electron irradiation of an oxide [1], a "non-stoichiometric climb model"

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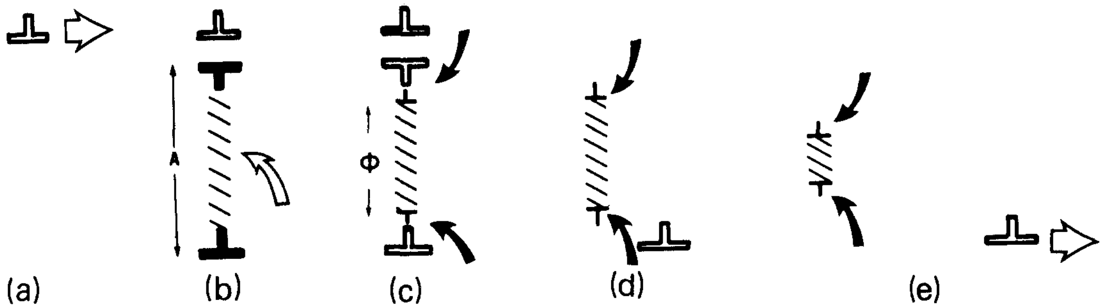

Figure 1 The different steps of the non-stoichiometric climb model (for details see text). White arrows: diffusion and aggregation of the faster ion. Black arrows: diffusion of the slower ion.

of dislocation, extended to the plasticity of oxides, is suggested. It is emphasized that the description of the climb model which is developed in this paper is a phenomenological hypothesis and is therefore schematic. All the assumptions suggested in this work are open to discussion.

2. Non-stoichiometric climb model

The following climb model is based on the different behaviours of the oxide components. The description is developed through the example of a binary oxide, the yttrium oxide (Y_2O_3) where the faster component is oxygen. Furthermore, a large concentration of oxygen interstitials may be present in the matrix. Nevertheless, the description is not confined to this material.

The climb model may be divided into the following stages:

(1) a gliding dislocation is stopped by an obstacle, for instance impurities or small clusters (Figs. 1a, 2a). Fig. 2a shows a very simplified picture of a gliding edge dislocation core in Y_2O_3 with 8 extra-half planes;

(2) the faster ions, oxygen in our example, diffuse to or along the dislocation and aggregate to form clusters in the lower part of the extra-half planes (Figs. 1b, 2b). The proximity of both dislocation and impurities may aid such a nucleation

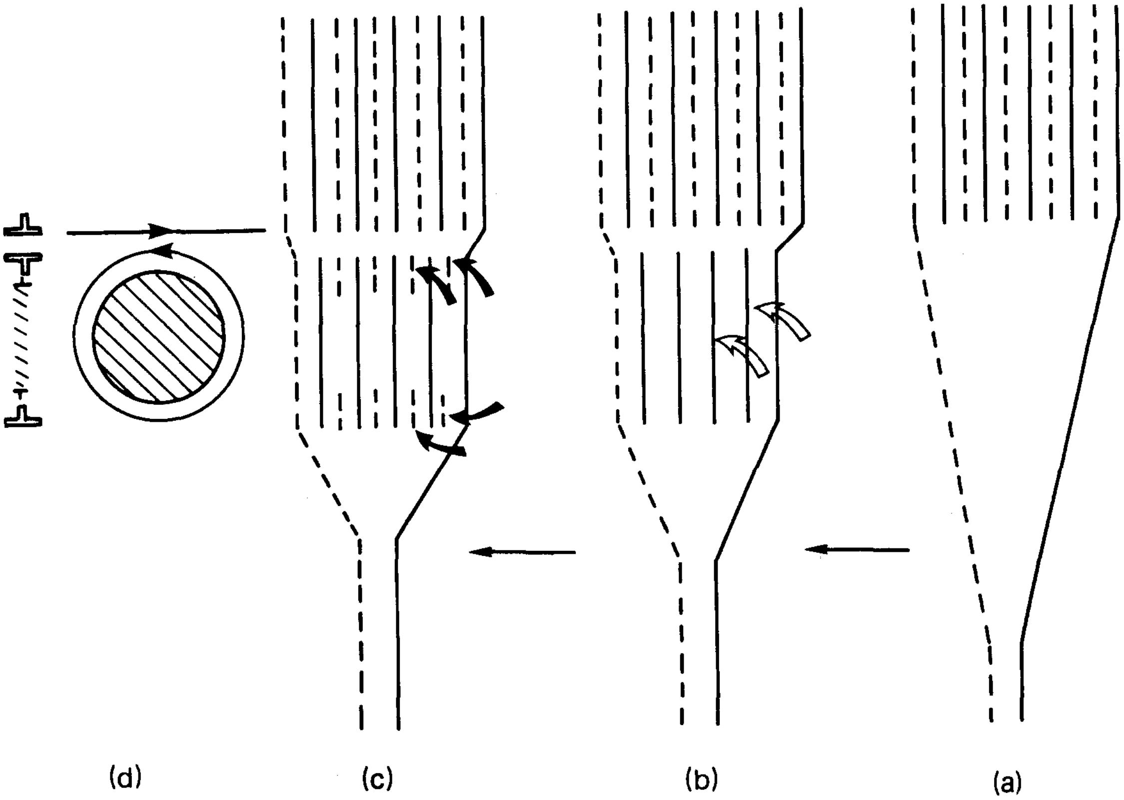

Figure 2 Schematic view of the climb mechanism.

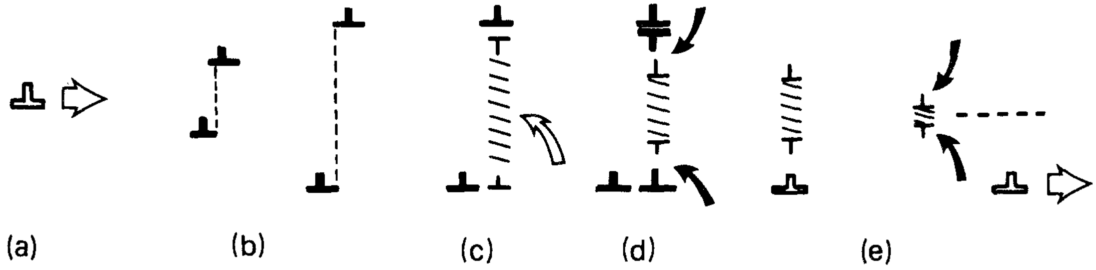

Figure 3 Non-stoichiometric climb mechanism applied to the unpinning process of a dislocation dissociated by climb (white and black arrows: as in Fig. 1).

process. Taking into account the core structure of the dislocation, this step could be rapidly achieved. In our example of Y_2O_3, this cluster nucleation may be suggested under the form of either neutral oxygen ions or molecule oxygen for electrostatic and ion size reasons. Such clusters are postulated to be coherent with the matrix or may be converted into more stable forms, such as a dislocation loop when they reach a certain size. Both considerations allow a description in terms of "interstitial dislocation loop". Experimental observations of irradiation defects support this hypothesis;

(3) the "interstitial dislocation loop' dissociates into two dislocations by transport of the slower ion, yttrium (Figs. 1c, 2c and d). A "crown" of perfect crystal is created between the two dislocation loops by the same process as that proposed for the irradiation defects;

(4) the initial dislocation reacts with the outer loop which has the same Burgers vector, but with the opposite sign, and then climbs (Fig. 1d);

(5) under the action of stress, the dislocation could glide again and leave behind "interstitial loops" (Fig. 1e).

It is worth noting that the yttrium transport to the residual loop may continue and result in their total disappearance (Fig. 1e). This slow shrinking process is independent of the unpinned dislocation motion. Thus dislocation can: (1) overpass such local obstacles as impurities or small clusters; (2) wholly climb by a succession of such mechanisms along the dislocation line.

Compared with the classical "stoichiometric climb model", this model shows the following differences: (1) the climb process is triggered by the components of the oxide which diffuse faster in the vicinity of the dislocation; (2) the slower ions intervene in the formation of a narrow perfect crystals "crown" which leads to the dissociation (Fig. 1c and d). This local process may be considered as faster than the process involving transport of stoichiometric matter to the dislocation.

This climb model may be considered as a series-type process. Two main mechanisms are interdependent.

(1) The first step is the non-stoichiometric transport of matter which leads to the "interstitial loop" nucleation (Fig. 1b). Let us suppose that the average velocity of this step is V_A and its duration is t_A. The characteristic length is then the diameter of the faulted loop: A (Fig. 1b).

(2) The second step is the reconstitution of a perfect crystal "crown" on the other rim of the "interstitial loop" which leads to dissociation, combination, and then to the climb of the initial dislocation. Let us suppose the average velocity of this step to be V_B and its duration t_B. The characteristic length of this step is B, with $B = A - \phi$, ϕ being the diameter of the remaining "interstitial loop" (Fig. 1c).

At the end of the whole mechanism, the climb distance is A and the surface virtually swept by the climbing dislocation is approximately $S \simeq \pi A^2/4$. The average climb velocity is V_c. The duration of climb is t_c. The following relation may be written:

$$t_A = \frac{A}{V_A}; t_B = \frac{B}{V_B}; t_c = t_A + t_B = \frac{A}{V_c}$$

the climb velocity is then:

$$V_c = \frac{A V_A V_B}{A V_B + B V_A}$$

or

$$V_c = \frac{V_A}{1 + (B/A)(V_A/V_B)} = \frac{V_B}{(V_B/V_A) + (B/A)}.$$

Other sites are favourable to the nucleation of such a climb mechanism, e.g. in the case of stacking fault ribbon. Let us take the example of dislocation dissociated by pure climb, i.e. climb splitting only proceeds from ionic diffusion from one partial to the other (Figs. 3a and b and 4a). Such a dislocation

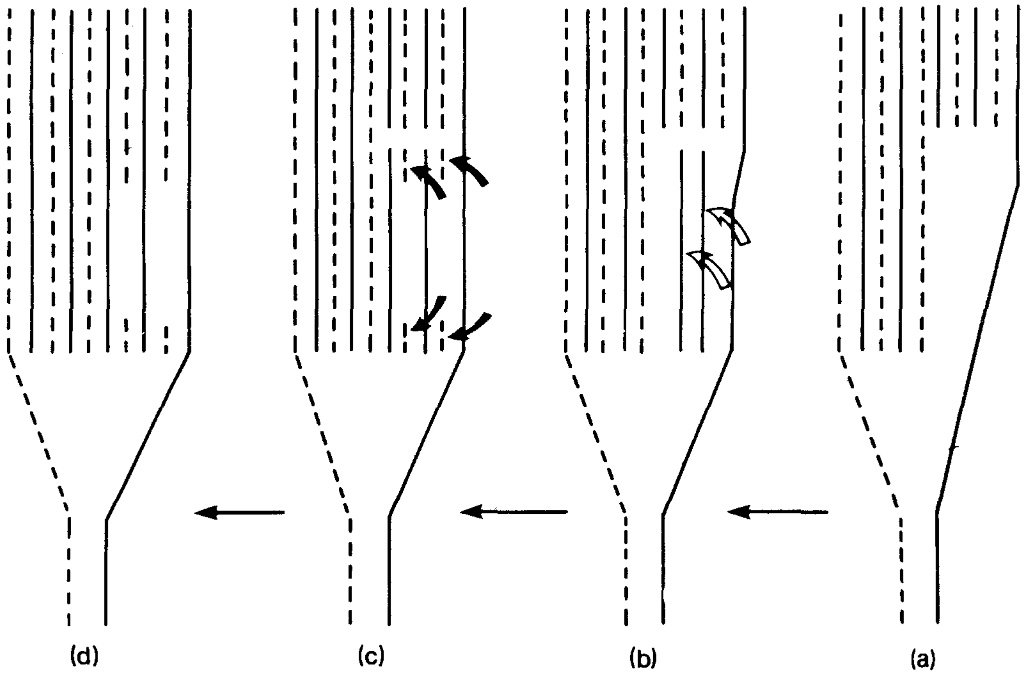

Figure 4 Schematic view of the unpinning process described in Fig. 3.

is sessile. The non-stoichiometric defect (Fig. 1b) may nucleate on the stacking fault ribbon, i.e. in the prolongation of the extra-half plane of one of the partial dislocations (Figs. 3c, 4b). A similar mechanism to the one described above, leads to the constriction of the climb dissociated dislocation.

Following the linear extension of this phenomenon, such a climb mechanism could lead to the unpinning of the sessile configuration. Assuming there is the aid of the applied stress, the dislocation may escape from the sessile configuration and start gliding again (Fig. 5).

3. Discussion

According to the expression of V_c, several cases may be considered.

$$V_A \gg V_B \Rightarrow V_c \simeq V_B \frac{A}{B} \tag{1}$$

$$A/B = 1 \Rightarrow V_c = V_B \tag{1a}$$

This case corresponds to the whole reconstitution of the perfect crystal inside the "interstitial loop". It is, in fact, the classical stoichiometric climb model which is controlled by the slower step.

$$B \ll A \Rightarrow V_c \simeq V_A \left(\text{if } \frac{V_B}{V_A} > \frac{B}{A}\right); \tag{1b}$$

this case is particularly interesting because the first step is the fastest ($V_A \gg V_B$) and because only a narrow "crown" of perfect crystal is needed for the dissociation. Those assumptions are motivated by the observation of irradiation defects. The climb velocity corresponds to the velocity of the

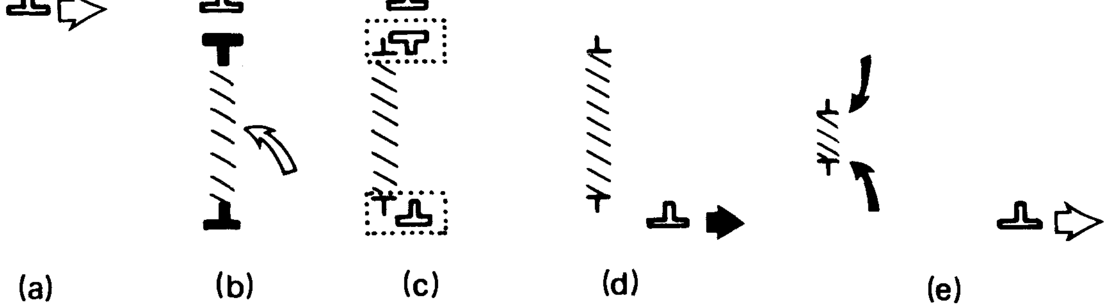

Figure 5 Possible steps of the unpinning process of a dislocation dissociated by climb.

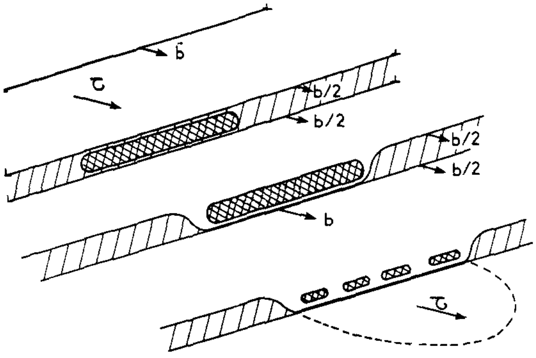

Figure 6 Non-stoichiometric climb mechanism involving "glide decomposition" (see text).

faster step. Furthermore, at the border line case $B = 0$, a "glide decomposition" induced by an applied stress may be suggested [2] (Fig. 6). In this later case, the second component of the binary oxide does not intervene in the dislocation unpinning process.

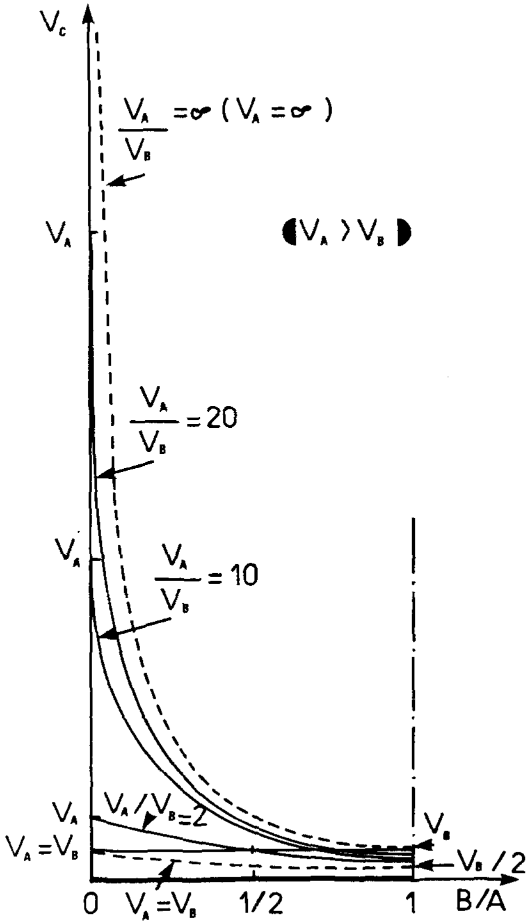

Figure 7 Climb velocity versus the B/A ratio for $V_A > V_B$.

$$V_A = V_B \tag{2}$$

$$A/B = 1 \to V_c = V_{A/2} = V_{B/2} \tag{2a}$$

$$B \ll A \to V_c = V_A = V_B \tag{2b}$$

$$V_A \ll V_B \tag{3}$$

$$A/B = 1 \to V_c \to V_A \tag{3a}$$

The slower step controls a process similar to the classical mechanism of climb ($B = A$).

$$B \ll A \to V_c \Rightarrow V_A \tag{3b}$$

This discussion is summarized in Figs. 7 and 8.

This simple picture of a non-stoichiometric climb model makes the description in terms of activation energies, quite difficult. Obviously, it is not possible to speak only in terms of point defect absorption or emission to or from the dislocation. Other parameters may play an important role in the rate-controlling climb mechanism. It is the case, for instance, of the nucleation energy of a cluster having a critical size from which it will be possible to speak of a dislocation loop. Further growing of this cluster is made possible not only

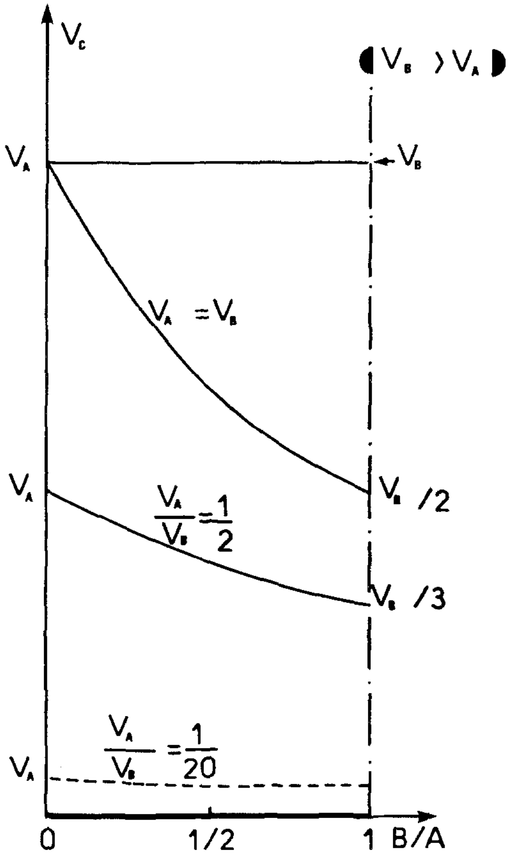

Figure 8 Climb velocity versus the B/A ratio for $V_B > V_A$

by diffusion but also whenever the corresponding "stacking fault energy" allows such an evolution. In fact the phenomenon resulting from the modification of the defect configuration must always be lumped in with a pure diffusion one.

Owing to these reasons, activation energy of plastic deformation controlled by such a climb model, might be quite different compared with those deduced from bulk diffusion of the slower component of the oxide or even from an effective diffusion coefficient taking into account the two species. The main interest of this climb model corresponds to Equation 1b. Faster diffusion of one of the components of the oxide, oxygen in Y_2O_3, and a large oxygen interstitial concentration due to the equilibrium with the environment leads to an extremely fast first step. Dissociation of the nucleated "interstitial loop" and the combination with the initial dislocation did involve a small amount of the second component which here is yttrium. Climb velocity would be then equal to the velocity of the fastest step. The lower diffusing ion, therefore, plays only a very small part.

4. Conclusion

In summary, it is thought that this climb model, which is a phenomenological hypothesis prompted by the reasons above, might play a role in oxide plasticity. A non-stoichiometric process is involved. Although this model is developed through the example of a binary oxide, the extension to more complicated material is possible. The first nucleation step might then be due to the faster diffusion and/or aggregation of an "ionic molecule" rather than to the behaviour of one of the components of the oxide.

References

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