INFLUENCE OF GRAIN BOUNDARY SPECIALNESS CHARACTER ON GRAIN TEXTURE AND BOUNDARY TEXTURE IN NICKEL OXIDE SCALES.

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INTRODUCTION

Many properties of polycrystalline materials depend on the characteristics of the grain boundaries\(^1\). More specifically, special grain boundaries, corresponding to some discrete intercrystalline misorientations (and to specific grain boundary plane orientations), preserve a good crystallographic fit between both adjacent crystals. Such interfaces have remarkable properties. In particular, special boundaries have a low energy in relation to general boundaries (Fig. 1), which turns them more stable than their general counterparts.

![Figure 1. Relative energy (\(\gamma_B/\gamma_s\)) of [001] and [011] NiO symmetrical boundaries versus misorientation\(^2\).](image)

\(^1\) Reference 1
\(^2\) Reference 2
The purpose of this study is to decide whether the preferred existence of special grain boundaries may promote crystallographic textures such as a grain texture, or a grain boundary texture, during the grain growth process, in NiO polycrystalline scales obtained by high temperature oxidation of nickel. If special boundaries play a significant role, their proportion may be expected to change in relation to that one expected in a random distribution of crystals as a function of the oxidation or annealing time. In order to check such a possible evolution, about 250 boundaries belonging to 6 samples have been studied by T.E.M. to determine:

- The geometrical orientation of the boundaries, to characterize the microstructure of the scales;

Figure 2. Boundary distributions versus tilt angle in relation to the surface of each scale (the oxidation and possible complementary annealing conditions are indicated in each distribution).
- The crystallographic orientation of the boundaries, to characterize the grain boundary texture;
- The crystallographic orientation of the grains, to characterize a possible grain texture;
- The intercrystalline orientation relationships, to classify the boundaries, and to distinguish between general and possibly special boundaries.

The methods which were used to collect the 3 first sets of data have been summarized elsewhere and the problems related to the determination of the possible special character of each boundary have been analyzed in full detail in 2 papers. I will just recall here that, when comparing the Coincidence Site Lattice (CSL) and Plane Matching (PM) crystallographic models of boundaries, it can be shown that any special CSL boundary such as $\Sigma<21$ and $\Sigma \neq 15$ is automatically a special (hkl) PM boundary [with $(hkl) = (111)$, $(002)$ or $(022)$], although the reciprocal is not systematically true. Finally, if the boundary population is split up into several sets, the hierarchy of these sets is as follows:
1) The boundaries really endowed with special properties belong to the CSL boundary set.
2) This set belongs, with few exceptions, to the PM boundary set.
3) The PM set belongs to the general boundary set.

Thus, the PM model appears of limited interest since it gives the same global information that the CSL model, but with a noise much more important, and an obvious lack of selectivity, vis-à-vis of the low angle boundaries especially. These are the reasons why, in the following, I will only consider the CSL model.

RESULTS AND DISCUSSION

Microstructure

As mentioned earlier 6 samples have been studied by T.E.M., and their microstructure characterized by determining the geometrical orientation of the grain boundaries in relation to the surface of each scale. The first sample (Fig. 2) is characterized by 2 sets of boundaries respectively perpendicular and tilted by about 40° in relation to the plane of the scale, which is typical of a non-random equiaxed microstructure. Reversely, the other 5 samples have just one set of boundaries roughly normal to the surface, which means that their microstructure is essentially columnar.

These observations are easy to interpret if it is keep in mind that NiO oxide scales have a dup-
lex structure, equiaxed close to the nickel-oxide interface, and columnar elsewhere. Thus, the first sample is representative of the area close to the nickel-oxide interface of the scale, and the others from the outside part.

Grain texture

The orientation distribution of the grains in relation to the surface of each scale (Fig. 3) suggests that some samples present a preferential orientation, but there is neither any consistency, nor any logic evolution of the texture of these samples as a function of the annealing time and annealing temperature. Quite likely, the apparent

Figure 3. Orientation of the grains in relation to the surface the scales.
texture which seems detectable in some cases results from a poor statistic and does not reflect the existence of a well established grain texture.

Grain boundary texture
The homogeneous distribution of the crystallographic orientation of the boundary planes (Fig. 4) shows that there is not any grain boundary texture.

Figure 4. Distribution of the crystallographic orientation of the boundary planes with location of the special boundaries (low angle boundaries are not represented).
Proportion of special boundaries

| Boundaries | Special Boundaries $\Sigma \in [3,25]$ |
|------------|--------------------------------------|
| number     | %                                    |
| 259        | 20                                   |
| 7.7 ± 4    |                                       |

Random distribution (Warrington & Boon) 9 ± 3

Special boundaries

If we consider that all the boundaries form only one homogeneous population, which is justified by the absence of grain and grain boundary textures, the proportion of special boundaries is exactly the same as that one expected in a random distribution of crystals (Table). This constatation is confirmed if we look more in detail to the distribution of the special boundaries (Fig.4). Nearly all the special misorientations are present, but in proportion close to that one expected in a random distribution. This observation is of special interest in the case of the $\Sigma 3$, 9 and 11 special boundaries, whose very low energy and actual special character have been experimentally confirmed, for symmetrical tilt boundaries (Fig. 1), whereas such actual low energy configurations were only observed in the case of one $\Sigma 11$ boundary (Fig. 4).

CONCLUSION

It appears clearly that the specialness character of the boundaries does not play any role, as regard to the textures, during the grain growth of NiO scales. This conclusion is valid whatever the microstructure is: equiaxed or columnar.

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