ATOMIC STRUCTURE OF AN fcc-HEXAGONAL INTERFACE

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Résumé - L'interface entre une matrice cubique à faces centrées et des précipités hexagonaux a été étudiée dans un superalliage par microscopie en faisceau faible et par haute résolution. L'alliage contenant une proportion importante de cobalt, la structure de la seconde phase est hexagonale ordonnée. Les précipités ont une forme de plaquettes parallèles aux plans compacts de la matrice. L' interface est elle même située dans ces plans. Le misfit entre les 2 phases est de 2 %. 3 familles de dislocations coins de vecteurs de Burgers 1/6<112> sont présentes. Ce réseau est triangulaire et possède la particularité de présenter des noeuds à 6 segments de dislocations. Les clichés de microscopie à haute résolution montrent que chaque dislocation est associée à une marche haute de 2 plans atomiques 111. Un modèle géométrique simple identique à celui d'un joint de torsion a été élaboré et rend compte de la géomètrie observée.

Abstract - The structure of the interface between fcc matrix and hexagonal precipitates in a superalloy has been studied using weak beam dark field and high resolution electron microscopy. An important percentage of cobalt is present in the alloy leading to an ordered hexagonal structure of the precipitates. They are plate-like shaped and the interface is parallel to the compact planes of both phases. There is a 2 % misfit between matrix and precipitate. The interface is made of 3 sets of 1/6<112> edge dislocations. These dislocations form a triangular net with nodes common to 6 segments of dislocations. Each dislocation is associated with a 2 atomic plane step. A simple geometric model identical to that of a twist boundary is presented.

1 INTRODUCTION

In a two phase alloy, the interface between the different phases play an important role in the different physical properties of the alloy. The knowledge of the structure of these interfaces is then necessary and it represents the first step in the understanding of the deformation process. Many different systems have been investigated on the experimental as well as on the theoretical point of view : Cu-Cr /1,2,/ , Al-Ag /3,4/. A review of the general problem of fcc-bcc interfaces can be found in ref /5/. In this kind of interfaces, the two phases have generally different crystallographic structure and different atomic parameters so that the situation is much more difficult than for the grain boundary problem where atomic models have been calculated and compared to experimental structure /6/. In this paper, an interface between fcc matrix and ordered hexagonal precipitates is investigated using weak beam dark field and high resolution electron microscopy.

2 EXPERIMENTAL PROCEDURE

2.1 Composition of the alloy and thermal treatments. The alloy was elaborated from very pure materials and the composition, in atomic percentage, is :

Co 37.6 Ni 36.8 Cr 22.5 Nb 3.1

so that the alloy composition is intermediate between Ni and Co based superalloys. It was obtained by melting the components under vacuum. The ingot was first annealed 6 h at 1250 °C under argon atmosphere. After this treatment, all the elements form a so solution. A second annealing treatment performed between 700 and 850 °C and from 24 120 h leads to the precipitation of a second phase which is responsible for the mechani properties of the alloy.

2.2 Electron microscopy. After thinning, the specimens are observed in a JEOL 4000 EX microscope. The resolving power of this microscope being around 1.7 Å /7/, the 111 (2 and 200 (1.8 Å) matrix planes are easily imaged.

3 RESULTS

3.1 Alloy morphology. After a 24 h incubation period, precipitates appear within matrix. They are plate-like shaped and the analysis of the diffraction patterns and of traces show that 4 orientation variants are present and that the broad faces of precipitates are parallel to the 111 compact matrix planes.

3.2 Crystallographic structure of the second phase. Chemical microanalysis of precipitates leads to the formula /8/:

$$(Co_{0.36}\ Ni_{0.61}\ Cr_{0.03}\ )_3Nb$$

Their structure is deduced from the analysis of the diffraction patterns and of the h resolution images taken on extracted precipitates. This structure is ordered hexagonal type. This particular structure is due to the presence of cobalt in large proport within the precipitates. In alloys containing only Ni, Cr and Nb, the precipitates have orthorhombic structure (β Ni_3Nb)/9/. These 2 structures are very similar, the c difference being the distribution of Nb atoms in the compact planes: in the DO_{19} struct it is triangular while in the orthorhombic it is rectangular. This phase change car explained in terms of conduction electron density /8/.

The matrix-precipitate orientation relationship is :

$$(0001)_p // \{111\}_m \text{ et } \langle 11\bar{2}0\rangle_p // \langle 110\rangle_m$$

This orientation relationship is a common one indicating that the compact planes compact directions of both phases are respectively parallel.

3.3 Structure of the interface. Fig 1 shows a weak beam dark field image of a sir interface observed nearly perpendicular to the interface plane. The diffraction vector <422> and 3 sets of dislocations are present; they form a triangular lattice and periodicity of this lattice is 100 Å . Contrast analysis using different diffract vectors showed that the dislocations are pure edge with a/6 <112> Burgers vectors v referred to the matrix.

When the matrix has a <011> orientation 2 sets of precipitates are seen edge-on. 1 orientation is the best one for high resolution observations because the compact planes both structures and the interface are in the edge-on position. If defocus conditions suitably choosen, the stacking sequence of fcc and hexagonal lattices are correctly ima so that the interface position can be accurately determined. The weak beam images sh that the interface structure consists in a triangular net of edge dislocations. Th dislocations lines are parallel to the three <011> directions lying in the interf plane.

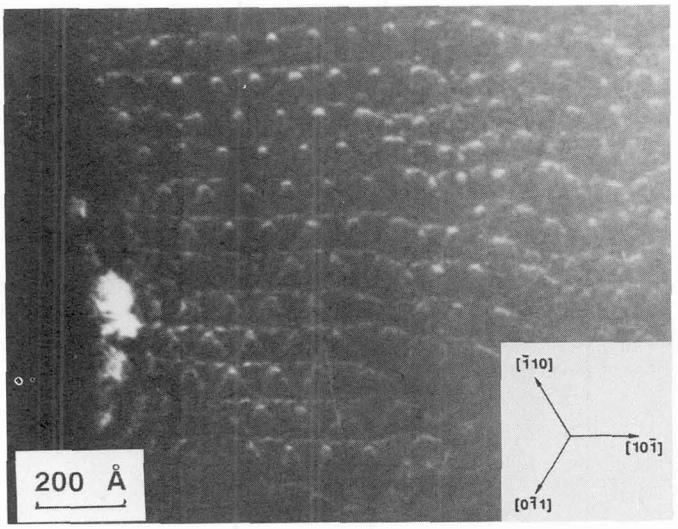

Fig 1 : Weak beam dark field image of a single interface nearly perpendicular to the incident beam. The dislocation network has a triangular distribution ; 6 dislocation segments meet at the nodes. The Burgers vectors are 1/6 <112> (when referred to the matrix).

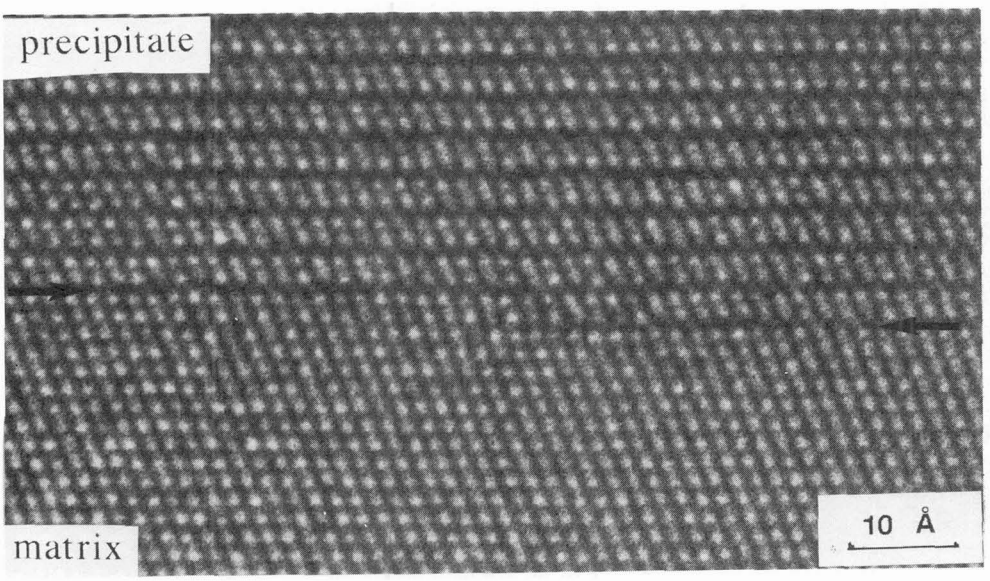

Fig 2 : High resolution image of the interface. In this orientation, the stacking sequence of both phases are imaged. The position of the interface is arrowed on both sides of an interfacial dislocation

With the orientation used for high resolution images, only one set of dislocations parallel to the incident beam, the 2 other ones being inclined. This is not a convenient situation but in thin parts of the specimen (the thickness must be less t 100 Å), images of interfacial dislocations have been obtained (fig 2). The Burg vectors and the interface position can be determined from these images. Two differ Burgers vectors were found. The first one corresponds to the edge a/6 [11$\bar{2}$] vector wh is parallel to the image plane; in this case 2 extra half atomic planes perpendicular the interface are present. The second Burgers vector is equal to a/12 [11$\bar{2}$] and corresponds to the projection on the observation plane of the inclined a/6 [$\bar{1}$2$\bar{1}$] Burg vector(fig 3) so that the high resolution images are in agreement with the previous w beam dark field images. This inclined Burgers vector is only observed in extremely t parts of the specimen where the effects of the inclined dislocation line on the image be neglected. All the dislocations are associated to a step in the interface plane : 2. The step height is 2 d_{111} matrix planes but in some cases, mainly near the end of precipitates it can be larger.

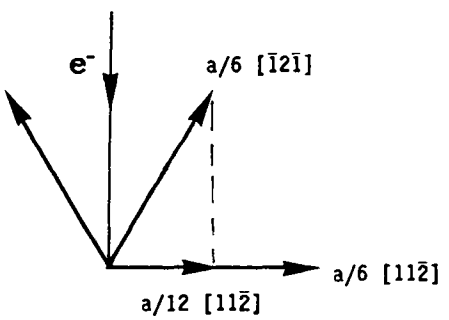

Fig 3 : Schematic diagramm showing the distribution of the different Burgers vectors wi respect to the incident electron beam. The 111 interface plane is parallel to the plane of the diagram.

4 INTERPRETATION OF THE RESULTS

The interfacial dislocation structure is governed by the symmetry of the system and by misfit between the atomic parameters of both phases.
The misfit is defined by :

$$\delta = 2\,\frac{d_m - d_p}{d_m + d_p}$$

where d_m and d_p are respectively the atomic parameters of the matrix and the precipitat It can be measured directly on the electron diffraction patterns and the value is :

$$\delta = 0.019$$

Using the Bollmann's formalism /10/, a coincidence site lattice (CSL) can constructed. The compact planes of both phases have a 3 fold symmetry and the dense ato rows are parallel so that the CSL has the same geometry : fig 4a. Its parameter depends the misfit; with the previously δ calculated value this parameter is 130 Å which is lar

than the experimental distance between dislocations. The simplest possible dislocation structure is shown on fig 4b. Each dislocation segment lies between two adjacent good fit areas. The result is an hexagonal network of a/2 <110> edge dislocations which is not in agreement with the experimental images. This structure has however been observed in some Ni base superalloys /11/. It also corresponds to the structure of twist grain boundaries in metals /10/. From this analogy with a twist boundary, other geometrical models can be constructed if some dislocation nodes are allowed to dissociate. This procedure has been described in detail by Hirth and Lothe /12/. The dislocation nodes can be separated into 2 different classes: K and P and in each class the nodes can be symmetrical or unsymmetrical. If only the P nodes dissociate, the structure shown in fig 4c results. The dislocations are now partial edge dislocations (b = a/6<112>). Their distribution is triangular and 6 dislocation segments meet at each node. The spacing between dislocation is 110 Å. It should be remarked that in the case of a twist boundary, the dissociated nodes correspond to an intrinsic stacking fault and the dissociation amplitude is governed by the stacking fault energy.

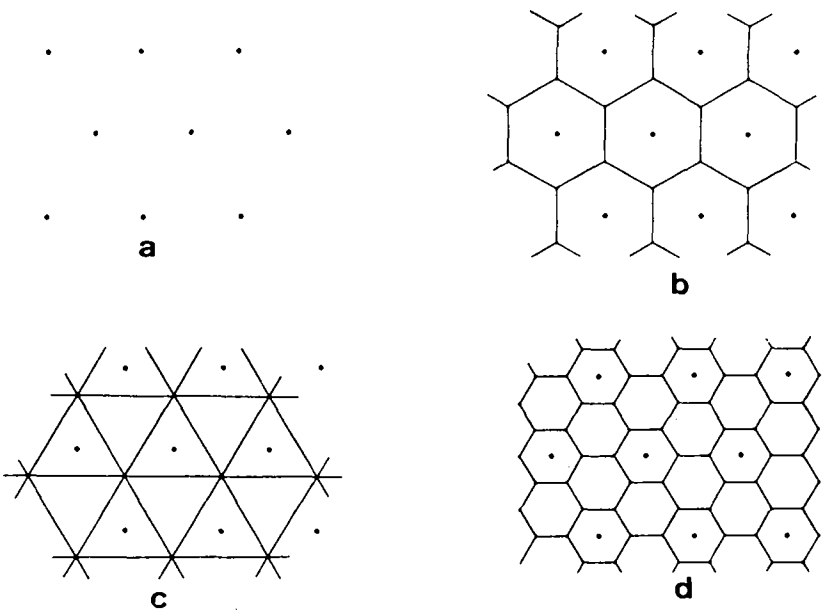

Fig 4 a - coincidence site lattice. The dots represent the centers of the good fit areas. The lattice has the same 3-fold symmetry as the compact planes of both phases. Its parameter is given by the misfit.

b - dislocation network deduced from the CSL.

c - dislocation network deduced from b when half the dislocation nodes are dissociated

d - same as c but all the nodes are dissociated.

In the interphase boundary, the stacking fault has no physical meaning but an equivalent situation exists if the interface plane moves towards a new good fit area which lies at a different level. This is why a two atomic step is associated to each partial dislocation. The necessity of such steps has already pointed out by King and Smith /13/ in rather similar examples. Finally, if both the P and K nodes can dissociate another structure is

possible which consists in an hexagonal network of partial dislocations. The spa between dislocations is now 75 Å : fig 4d. The comparison of the experimental image the interface boundary to these geometrical models shows that only the structure descr on fig 4c is possible.

5 CONCLUSION

Using weak beam dark field and high resolution electron microscopy, the structure of interface between an fcc matrix and hexagonal precipitates has been determined. geometrical misfit is relaxed by the presence of a triangular network of par dislocations. This rather unusual distribution can be described on the basis geometrical model using the CSL concept. The choice between the three different poss models is only made by comparison with experimental results and the final explanatio this particular structure will need the calculation of the energy of these configurati

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