CHARACTERIZATION AND MODELLING OF THE ANISOTROPIC MECHANICAL BEHAVIOUR OF NICKEL-BASED SINGLE CRYSTAL SUPERALLOYS FOR TURBINE BLADES

P. Poubanne*, P. Caron** and T. Khan**
* SNECMA-Villaroche, 77550 Moissy Cramayel, France
** ONERA, BP72 - 92322 Châtillon, France

Abstract

The nickel based single crystal superalloys are presently used as vanes and blades in some advanced gas turbine engines. For a more reliable and rational use of such materials an important requirement is the development of models allowing to predict the inelastic constitutive behaviour of such anisotropic materials. In the first part of this paper, we present the typical mechanical behaviours of representative single crystal superalloys. The creep behaviour of various alloys was investigated between 760 and 1050°C by varying the microstructure and the crystallographic orientation of the tensile axis. It is shown that the creep strength at 760°C and 750 MPa of CMSX-2 is strongly anisotropic, and that this anisotropy is very sensitive to the size of the strengthening γ' precipitates. At higher temperatures (950-1050°C), the effect of orientation on the creep behaviour of single crystal superalloys is still very significant. The tensile behaviour of single crystal superalloys is strongly dependent on the stress axis orientation. As the tensile strength of [001] and [011] crystals reaches a maximum around 760°C, it decreases continuously with increasing temperature in the case of [111] crystals. During the inelastic deformation stage, a much higher work hardening rate is observed for the [111] orientation than for the [001], while [011] crystals do not exhibit work hardening. In low cycle strain-controlled fatigue tests, and at least up to 950°C, the fatigue life of single crystal superalloys is dependent on cristallographic orientation of the stress axis. For a given strain range the fatigue life follows the pattern : [001] > [011] > [123] > [111]. This effect of orientation is essentially due to the anisotropy in elastic modulus. In the second part, a microphenomenological model developed for anisotropic single crystal superalloys is described and is shown to simulate fairly well both the monotonic and the cyclic mechanical behaviour at 950°C of AM1 single crystals with various crystallographic orientations.

I. Introduction

Nickel-based single crystal superalloys have only recently been introduced as turbine blade materials in some advanced US engines. In France, the advanced materials development work undertaken at ONERA in the early 1980's in collaboration with the engine manufacturers, SNECMA and TURBOMECA, led to the development of a number of new single crystal superalloys. Among the recent alloys, The AM1 [1], AM3 [2] and MC2 [3] alloys are worth mentioning. The AM1 alloy, for example, has been selected by SNECMA for use as vane and blade material in its advanced M88 military gas turbine engine, which will equip the RAFALE aircraft.

The turbine blade alloys in modern gas turbines must satisfy a set of property requirements. The airfoil must have a favourable combination of creep strength, thermal fatigue resistance and environmental resistance. The root section requires adequate monotonic and cyclic properties. Single crystal materials are highly anisotropic and hence it is important to characterize their mechanical behaviour along various cristallographic orientations in order to develop micro-phenomenological models. Indeed, from an industrial point of view, the aim is to predict WHEN and WHERE in a structure the damage will lead to the failure of the material under well-known mechanical and thermal loadings. Thus the knowledge of damage evolution implies first to determine the strain and stress fields in the structure for each time increment of the loading. The method often used is then the finite elements method. Nevertheless a basic need for this computation is the knowledge of the mechanical behaviour of the material. The results presented in the first part of this paper show that both elastic and inelastic behaviours of single crystal superalloys are highly anisotropic and that this anisotropy may depend strongly on the test temperature. Just about five years ago, no model was available to describe the elasto-visco-plastic behaviour for such materials. Driving by the aeronautical requirements, great improvements have been performed by scientists all over the world, in particular in France where two kinds of models have been developped for turbine blade design. The aim of these models is to simulate as much as possible the complex response of the material under complex mechanical loading.

Table 1 Nominal compositions (wt%) of the single crystal alloys.

Alloy	Origin	Ni	Cr	Co	Mo	W	Al	Ti	Ta
CMSX-2	USA	Bal.	8	4.6	0.6	7.9	5.6	0.9	5.8
AM1	France	Bal.	7.5	6.5	2	5.5	5.3	1.2	8

The purpose of this paper is, in the first place, to present some typical mechanical behaviours of representative single crystal superalloys in order to show how the metallurgical microstructure and the crystallographic orientation may affect their properties. In the second part, we will introduce the model which seems to be the most physically based, or at least, which may be improved by metallurgical considerations. This model requires, in particular, the identification of the active slip systems and the deformation mechanisms involved during the plastic flow and strain hardening of the material. We will show how this model can describe the monotonic and cyclic behaviour at 950°C of the single crystal superalloy AM1.

II. Anisotropic Mechanical Behaviour of Single Crystal Superalloys

Stress Rupture and Creep Behaviour.

A number of investigations have previously shown that the creep strength of single crystal superalloys around 760°C is highly dependent on orientation [4-6]. It was reported in the case of Mar-M 200 and Mar-M247 single crystals that there is a ranking in tensile creep strength : the highest lives were obtained near the [111] crystallographic orientation and the lowest near [011], [001] orientation showing intermediate in terms of strength. In these studies, however, no attention was paid to the combined effects of microstructure and orientation. It was therefore thought useful to undertake a detailed investigation of the anisotropic creep behaviour of some recently developed single crystal superalloys with well controlled metallurgical microstructure. The CMSX-2 alloy served as the base material for this investigation. The chemical composition of this alloy is

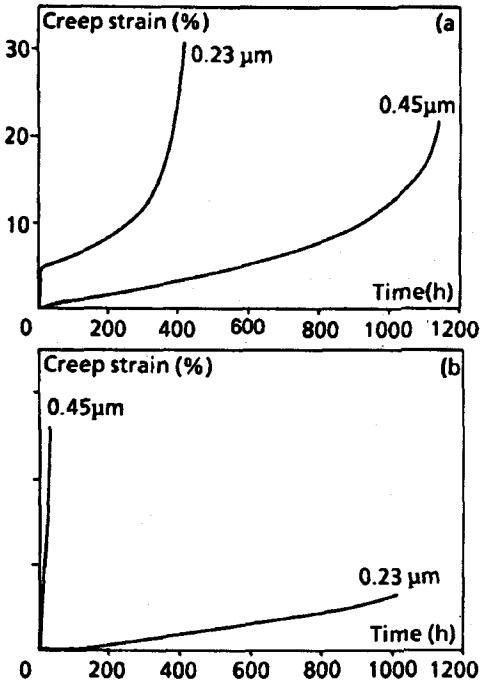


Fig. 1 Effect of γ' precipitate size and orientation on the creep behaviour at 760°C and 750 MPa of CMSX-2 single crystals : a) [001], b) [111].

reported in Table 1. The microstructure of the nickel-based superalloys consists of a face centered cubic γ matrix strengthened by a high volume fraction (up to 70%) of precipitates of the ordered γ' phase based on Ni_3Al. The precipitation heat treatments control the size and the distribution of the γ' particles. Two different precipitation heat treatments were applied to specimens of the CMSX-2 alloy, resulting in γ' sizes of 230 and 450 nm. The creep curves obtained at 760°C and 750 MPa with these two different microstructures for the [001] and [111] orientations are shown in Fig. 1.

For the [001] orientation, which is the natural growth direction of the single crystal blades, the longest lives are obtained with the largest precipitates. The reason for this is the extremely homogeneous nature of deformation resulting from the operation of {111}<110> multiple slip in the γ matrix during the early stages of deformation [7]. Reducing the γ' size from 450 to 230 nm promotes planar and heterogeneous deformation by extensive cooperative {111}<112> shearing of the γ and γ' phases. The overall result is a considerable increase in the amplitude of primary creep and a shorter rupture life for the [001] single crystals containing the smaller precipitates.

The [111] oriented crystals with a γ' size of 450 nm exhibit extremely poor creep strengths compared to the [001] single crystals having the same microstructure. Despite the fact that [111] is theoritically an orientation promoting multiple slip, careful analysis of the dislocation structure shows that the primary creep deformation takes place primarily by coplanar-slip in the γ matrix between the precipitates [7,8]. This deformation mode results in a weak strain hardening which explains the high creep rates observed in this case. For the near-[111] oriented single crystals, a reduction of the γ' size from 450 to 230 nm results in a 30-fold increase in the stress rupture life in spite of inhomogeneous {111}<112> deformation of the crystals containing the smaller particles. In fact, the resolved shear stress for the {111}<112> slip systems is smaller for a [111] stress axis than for a [001] one which therefore justifies the lower creep case shown in the former case even if the deformation is heterogeneous. These observations on the CMSX-2 alloy were confirmed on a number of other single crystal superalloys which showed the same

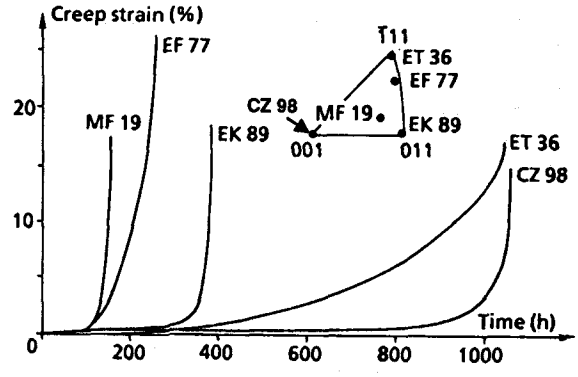


Fig. 2 Effect of orientation on the creep behaviour at 1050°C and 120 MPa of CMSX-2 single crystals (γ' precipitate size = 450 nm).

overall deformation features [8].

At higher temperatures, the anisotropy of the creep behaviour of the single crystal superalloys becomes much less pronounced but there can still be a factor of five in stress rupture lives even at a temperature of 1050°C [9]. This is illustrated in Fig. 2 where the creep curves of CMSX-2 single crystals containing precipitates with a size of 450 nm are shown for various selected orientations. The γ' size at this temperature does not have any significant effect on the anisotropic creep behaviour of the CMSX-2 alloy. The extremely low secondary creep rates for the [001] oriented crystals are because of the development of a rafted γ' morphology resulting from the oriented coalescence of the precipitates normally to the stress axis [10].

Tensile Behaviour

The tensile behaviour of CMSX-2 single crystals was investigated between room temperature and 950°C for the three main orientations [001], [111] and [011]. The tensile curves all exhibit a yield drop followed by an easy glide stage at room temperature and 650°C ; typical curves obtained at 650°C are shown in Fig. 3. The occurence of extensive easy glide in the temperature range 25-650°C of both [001] and [111] oriented crystals contrasts with the tensile behaviour of some earlier single crystal superalloys as Mar-M200 where the plateau region was only observed for single slip orientations near [011] [4]. At room temperature, tensile tests on prepolished plate specimens were interrupted during the plateau stage. Extremely localized heterogeneous slip bands were observed parallel to the primary octahedral slip plane [5]. The plateau region corre-

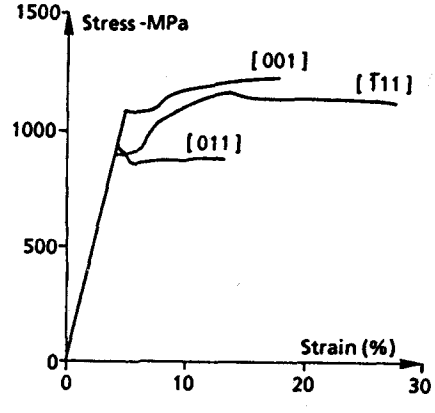


Fig. 3 Typical tensile curves at 650°C for CMSX-2 single crystals with different stress axis orientations.

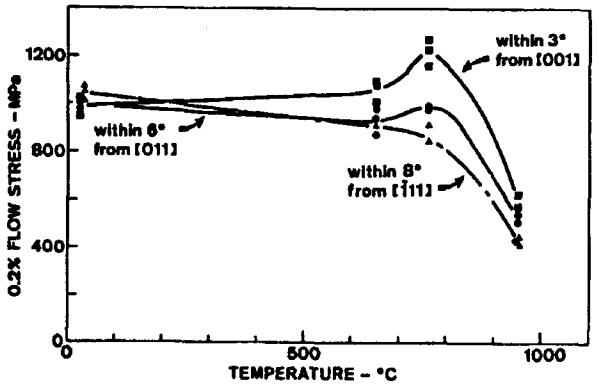


Fig. 4 Temperature dependence of the 0.2% flow stress of CMSX-2 single crystals as a function of orientation.

sponds to the propagation of such slip bands in the entire gauge length of the specimens. Analysis of the dislocation structure during this stage shows that the deformation is localized in narrow deformation bands were the γ' precipitates are cut by a<110> superdislocations [5]. For the [001] and [111] crystals, the plateau region is followed by a work hardening stage, but the [011] specimens fail in this region. These plastic instabilities observed during tensile tests in the modern single crystal superalloys can be of concern in the root section of the turbine airfoils, and therefore special attention should be paid to understanding the origin of such phenomenon.

The temperature dependence of the 0.2% flow stress as a function of the orientation of the stress axis is shown in Fig.4. At room temperature, the three orientations [001], [111] and [011] exhibit the same value of 0.2% flow stress. Then, the 0.2% flow stress reaches a maximum around 760°C for the [001] and [011] crystals, whereas it decreases continuously with increasing temperature for the near-[111] oriented specimens.

Fig. 5 shows the temperature dependence of the ultimate tensile stress (UTS) for CMSX-2 single crystals. At room temperature, the [111] specimens show the highest values of UTS, resulting from a very high work hardening rate. The lowest UTS is observed for the near [011] oriented crystals which are characterized by the absence of work hardening due to the operation of a single slip system. Relatively poor work hardening rates shown by the near [001]

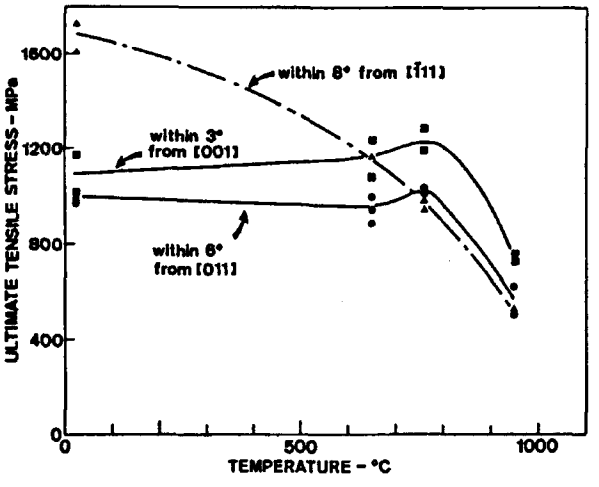


Fig. 5 Temperature dependence of the ultimate tensile stress of CMSX-2 single crystals as a function of orientation.

oriented specimens lead to UTS values which are much lower than for [111] crystals. As the temperature increases, UTS for the three orientations follows the same trend as that shown by the 0.2% flow stress.

The deformation modes operating during the tensile tests depend on the orientation of the stress axis. The nature and the number of activated slip sytems were determined by slip trace and transmission electron microscopy analysis on specimens strained to 2% [5]. Between room temperature and 950°C, [001] and [011] crystals deform by {111}<110> octahedral slip (multiple or single slip respectively) whereas [111] specimens deform by {001}<110> cube slip.

Low Cycle Fatigue Behaviour

Total strain controlled fully-reversed low cycle fatigue tests were performed at 650 °C on single crystal specimens of the AM1 superalloy which composition is reported in Table 1. The specimen stress axes were close to the orientations [001], [123], [111] and [011]. The number of cycles to rupture are reported as a function of the total strain range in Fig. 6a. For a given strain range the fatigue life follows the pattern : [001] > [011] > [123] >[111]. In fact, the plastic strain component in such alloys is small and therefore the results obtained with strain controlled tests can be very well plotted as a function of the total stress range as shown in Fig. 6b. In this plot, all experimental data fall on a single straight line which shows that the effect of orientation is essentially due to the strong anisotropy of Young's modulus of the single crystals. The value of the Young's modulus is minimum for [001] and maximum for [111], respectively close to 110 and 270 GPa at 650°C. Similar effects of orientation were observed at 950°C.

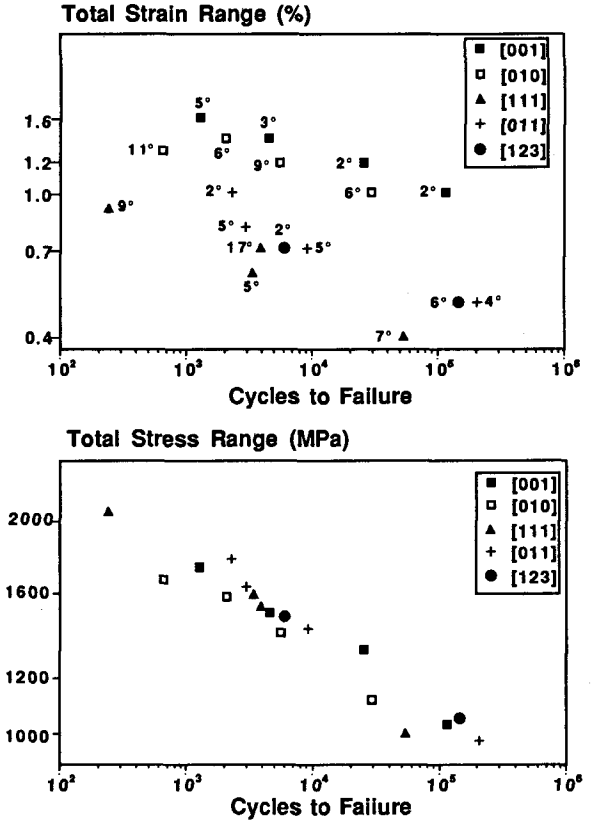


Fig. 6 Effect of orientation on the LCF behaviour at 650°C of AM1 single crystals (R = -1, frequency = 0.33 Hz). The degrees represent the departure from the main orientations.

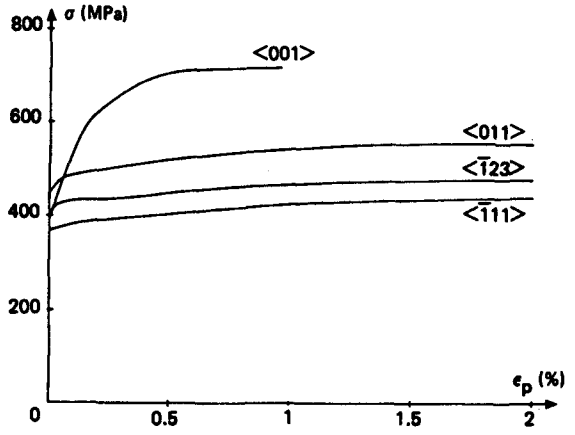


Fig. 7 Comparison of the monotonic tensile curves at 950°C of AM1 single crystals with various cristallographic orientation.

III. Modelling of the Anisotropic Mechanical Behaviour of a Single Crystal Superalloy

Experimental Tests

As a first step, in modelling the anisotropic mechanical behaviour of a single crystal superalloy, whe have tried to simulate the monotonic and the cyclic behaviour at 950°C of the AM1 alloy by using a model first proposed by Cailletaud [11].

Uniaxial tensile tests were conducted at 950°C on AM1 single crystals with stress axes oriented along [001], [011], [111] and [123]. The strain rate was $1.1.10^{-4}s^{-1}$. Typical tensile curves obtained for the different orientations are shown in Fig. 7. Since only their inelastic behaviour is considered, the experimental results are shown on a σ vs. ε_p basis.

In order to describe the cyclic behaviour of the AM1 alloy, we have taken into account the fatigue hysteresis loops of single crystals subjected to fully-reversed low cycle fatigue tests at 950°C. The specimens were tested in the total strain control mode with $R_\varepsilon = -1$ using a triangular waveform-signal. A typical cyclic stress-strain curve of a [123] single crystal is shown in Fig. 8. The cyclic hardening curves for the four orientations are compared in Fig. 9.

The main phenomenological features of these monotonic and cyclic behaviours are as follows :

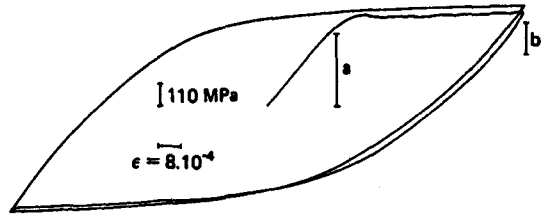


Fig. 8 Illustration of cyclic stress-strain curve at 950°C of a AM1 single crystal specimen oriented along <123> ($\Delta\varepsilon_T$ = 1.95%, t = 376 s). The initial elastic domain (a) is reduced to (b) at the first quarter cycle.

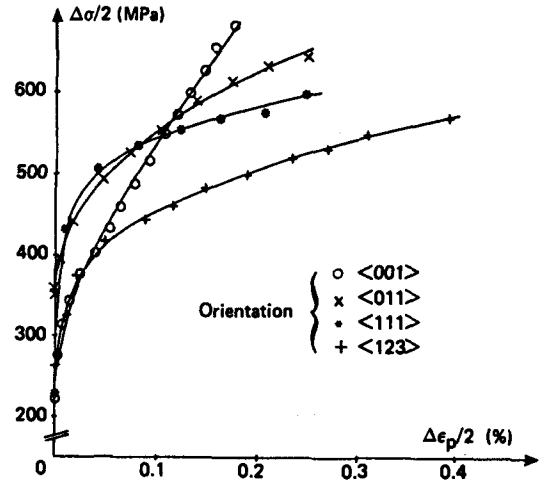


Fig. 9 Comparison of the cyclic hardening curves at 950°C of AM1 single crystals with various cristallographic orientations.

- the mechanical behaviour is strongly dependent on the crystal orientation , as in other tests,
- a strong strain-rate dependence is observed,
- both monotonic (Fig. 7) and cyclic tests (Fig. 9) show the highest hardening rate for [001] compared to the other orientations, and especially [111],
- a reversed loading after the first quarter cycle reveals a very fast reduction of the elastic domain. Therefore, the hysteresis loops have a pronounced kinematic character (Bauschinger effect) (Fig. 8).

By using transmission electron microscopy, it was possible to determine the nature of the slip systems activated during the plastic deformation at 950°C : the AM1 single crystals deform at 950 °C by the glide of dislocations on one or more of the twelve{111}<110> octahedral and six {001}<110> cubic potential slip systems. Each of these slip systems is defined by the directions n^g normal to the slip plane and b^g corresponding to the slip direction (g = 1, N with N = 18). Hardening originates from complex micromechanisms including interactions betweens dislocations themselves and interactions between dislocations and γ' precipitates [12]. At 950°C, the deformation takes place mainly in the matrix between the precipitates.

Microphenomenological Modelling

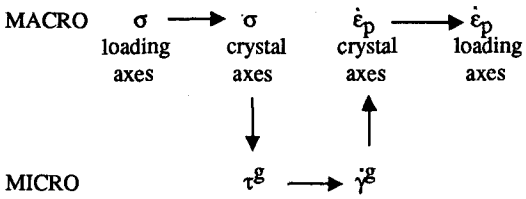
What occurs physically during shear on slip systems seems too complex to be directly simulated, but it is possible to describe the main effects of plastic shear γ^g on local (slip system) hardening owing to, what we call, internal variables. These variables are only supposed to describe the main "micromechanism" effects, but not the micromechanisms themselves. However, the choice of the type of internal variables to be considered should be inspired by the micromechanisms that are involved during the deformation process. Then the overall response of the material element can be deduced from the contribution of each slip system. This is the basic idea of the micro-macro modelling.

The introduced model was proposed by Cailletaud [11]. It takes into account the crystallographic nature of slip on both the octahedral and cube planes as observed in experiments. The constitutive equations are expressed at the slip system scale, in order to better describe the main effects of the microscopical mechanisms.

The first step is to express a local yied criterion for each slip system. At high temperature the Schmid's Law is a very good approximation. It stipulates that a slip system is active only if the re-

solved shear stress τ^g on the slip plane n^g towards the direction b^g becomes higher than a critical value τ_c^g which depends on the material and its inelastic strain history.

Inelastic shear strain rate on each active slip system contributes to the macroscopical inelastic strain rate tensor (with assumption of strain homogeneity). The relations are given in [13]. So the concept of micro-macro modelling may be summarized as follows :



with :

$$\tau^g = \frac{1}{2}(n_i^g b_j^g + n_j^g b_i^g)\sigma_{ij} = R_{ij}^g \sigma_{ij}$$

$$\dot{\varepsilon}_{ij}^P = \sum_{g=1}^{N} R_{ij}^g \dot{\gamma}^g$$

The constitutive law is then a relation between the resolved shear stress τ^g on the system g, and the viscoplastic shear strain rate $\dot{\gamma}^g$ on the same system. A basic assumption is that plastic shear strain is the cause of hardening and changes the value of τ_c^g. For phenomenological and even metallurgical reasons [12], the evolution of τ_c^g is decomposed in two hardening variables. The first one represents isotropic hardening r^g : expansion or vanishing of the elastic domain, the second one x^g : rigid translation of the elastic domain in a stress space. These two variables include respectively the elastic domain vanishing, and the reversed loading effects.

The evolution laws during the deformation process are given as follows :

$$dx^g = c_j(a_j\Phi(v^g)d\gamma^g - x^g|d\gamma^g|) \quad \text{with} \quad \Phi(v^g) = \Phi_j^{\infty} + (1-\Phi_j^{\infty})\exp(-\delta_j v^g)$$

$$dr^g = \sum_{s=1}^{N} b_j H(g,s) Q_j \exp(-b_j v^s)|d\gamma^s| \quad \text{with} \quad v^s(t) = \int_0^t |\dot{\gamma}^s| dt$$

where j takes the value 1 or 2 respectively for octahedral and cube slip, which means that two families of material coefficients are needed.

The important points are :
- kinematic variable evolution on slip system g is assumed to depend only on the shear strain on the slip system itself,
- a non linear evolution, with accumulated strain history effect, is used for x^g,
- isotropic variable evolution on slip system g is assumed to depend on inelastic shear strain produced on this sytem as well as on every other potential slip system,
- the term H(g,s) of the "interaction matrix" allows to introduce the cross influence of the slip system s on the isotropic hardening of the system g. Diagonal coefficients describe the self-hardening which can be an hardening or softening effect according to the Q_j value ($Q_j > 0$ = hardening, $Q_j < 0$ = softening). Cross-hardening effect is taken into account through h (for weak interactions) and q (strong interactions) coefficients, which give finally the following 18x18 interaction matrix expression :

H(g,s)

1	h	h	h	q	q	h	q	q	h	q	q	0	0	0	0	0	0
h	1	h	q	h	q	q	h	h	q	q	q	0	0	0	0	0	0
h	h	1	q	q	h	q	q	h	h	q	q	0	0	0	0	0	0
h	q	q	1	h	h	h	q	h	q	q	h	0	0	0	0	0	0
q	h	q	h	1	h	q	h	q	q	h	q	0	0	0	0	0	0
q	q	h	h	h	1	q	q	h	q	q	h	0	0	0	0	0	0
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q	q	h	h	q	q	1	h	h	q	q	h	0	0	0	0	0	0
q	h	q	h	q	h	h	1	q	h	q	q	0	0	0	0	0	0
q	q	h	h	h	q	q	q	1	h	q	q	0	0	0	0	0	0
q	q	h	h	q	h	q	h	h	1	q	q	0	0	0	0	0	0
q	q	h	h	q	q	h	q	q	q	1	h	0	0	0	0	0	0
q	q	h	h	h	q	q	q	h	q	h	1	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	h	q	q	q	q
0	0	0	0	0	0	0	0	0	0	0	0	h	1	q	q	q	q
0	0	0	0	0	0	0	0	0	0	0	0	q	q	1	h	q	q
0	0	0	0	0	0	0	0	0	0	0	0	q	q	h	1	q	q
0	0	0	0	0	0	0	0	0	0	0	0	q	q	q	q	1	h
0	0	0	0	0	0	0	0	0	0	0	0	q	q	q	q	h	1

In a viscous framework, shear strain rate is given explicitely for each slip system by Cailletaud [11] :

$$\dot{\gamma}^g = \left\langle \frac{|\tau^g - x^g| - r^g}{K} \right\rangle^n \operatorname{sign}(\tau^g - x^g)$$

Material's coefficients are then determined with the help of both the experimental data and calculations. This involves some further assumptions because test results only concern the mechanical behaviour of the material's element and not directly the slip system. Hence, the experimental data are analyzed by assuming equipartition of plastic strain for equi-loaded slip sytems (8 equi-loaded {111}<110> slip systems in a <001> perfectly oriented specimen in tensile test for example) which supply a first set for material's coefficient values. Then computer aided calculations permit to obtain a reasonable set of material coefficients.

The model's validity domain ranges from low to medium plastic strain rate and affects only small displacements. It means in particular that extremely localized heterogeneous slip bands appearing during deformation at low temperatures cannot be properly described. Only a mean homogeneous inelastic strain will be given in this case. An other restriction deals with the identification of the material's coefficients : they concern a given material with a given metallurgical microstructure. In some respects the microstructure is included in the model.

Figs. 10 and 11 show comparisons between experimental and predicted deformation curves illustrating the monotonic and cyclic behaviours of AM1 single crystals tested at 950°C. The model simulates fairly well the hysteresis loops obtained for four different crystallographic orientations during the low cycle fatigue tests (Fig. 10). Fig. 11 shows that the strain rate changes during the monotonic tensile tests can also be correctly simulated by using this model.

Conclusions

The various mechanical tests conducted on single crystal superalloys for turbine blades show that their elastic and inelastic behaviours are highly anisotropic and that in some cases (e.g. in creep) this anisotropy may depend on the test temperature and on the me-tallurgical microstructure. A new challenge for the designer is to develop models which allow to simulate the response of such anisotropic materials under complex mechanical loading. The

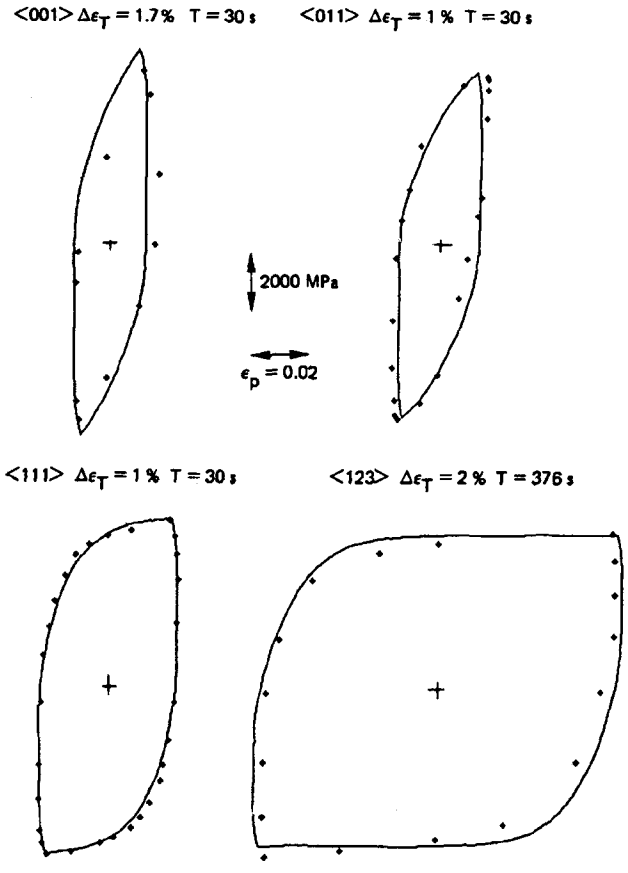

Fig. 10 Comparison between predicted and experimental hysteresis loops for four crystallographic orientations of the AM1 single crystal superalloys tested in low cycle fatigue at 950°C ; ++ : tests, —— : calculation.

microphenomenological model described here takes into account the nature of the microscopic mechanisms controlling the inelastic deformation. This model seems simple enough to be introduced in a finite element code without too much difficulties, but is flexible enough to simulate succesfully complex mechanical response of single crystal superalloys, at least under conditions where the inelastic strain is homogeneously distributed in the material. This work shows for instance that this model can simulate both monotonic and cyclic behaviours of AM1 single crystals at 950°C under uniaxial stress and for various crystallographic orientations. Such a modelling should be applicable in an industrial context, at SNECMA, in the near future.

Acknowledgements

The work concerning the modelling of the mechanical behaviour of the AM1 single crystal is a part of a doctoral thesis [12] carried out at Office National d'Etudes et de Recherches Aérospatiales (ONERA) in cooperation with Ecole des Mines de Paris, with the financial support of Société Nationale d'Etudes et de Construction de Moteurs d'Aviation (SNECMA).

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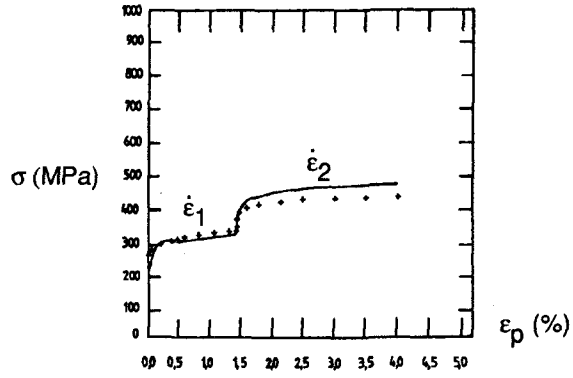
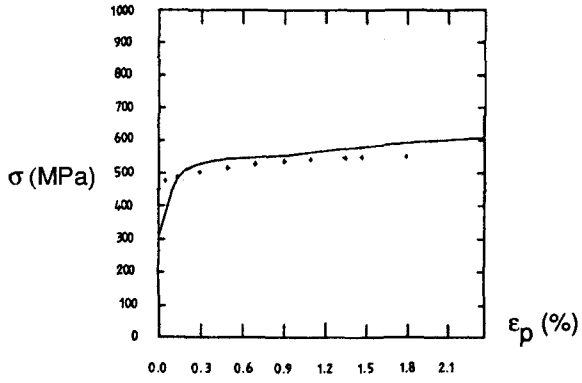
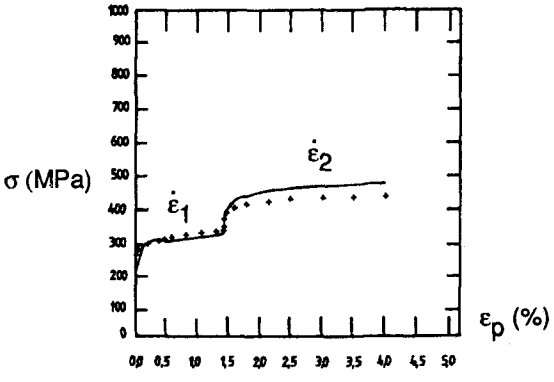


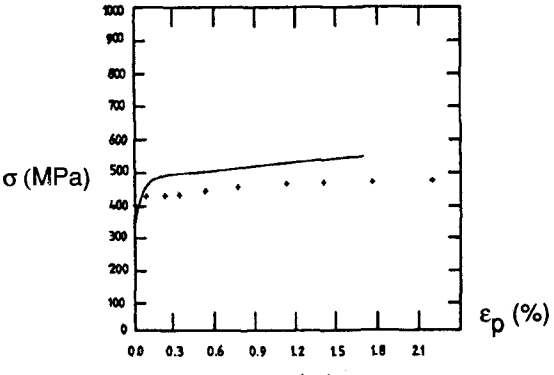
a) <001> stress axis ; $\dot{\varepsilon}_1 = 4.4.10^{-6}s^{-1}$, $\dot{\varepsilon}_2 = 10^{-4}s^{-1}$.



b) <011> stress axis ; $\dot{\varepsilon} = 1.1.10^{-4}s^{-1}$.



c) <111> stress axis ; $\dot{\varepsilon}_1 = 4.4.10^{-6}s^{-1}$, $\dot{\varepsilon}_2 = 10^{-4}s^{-1}$.



d) <123> stress axis ; $\dot{\varepsilon} = 1.1.10^{-4}s^{-1}$.

Fig. 11 Comparison between predicted (——) and experimental (+++) tensile curves at 950°C of AM1 single crystals with various orientations.

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