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Decorrelated Dislocation Movement in the γ-Matrix Channels of a Ni-Based Superalloy: Experiment and Dislocation Dynamics Simulation

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Abstract. The mechanical behavior of the polycrystalline NR3 Ni-based superalloy has been investigated at the microscopic scale. The elementary deformation mechanisms have been analyzed using transmission electron microscope observations as well as *in situ* straining experiments. Under low stress and relatively low strain rate conditions, a large variety of shearing micromechanisms has been observed depending on the local microstructure and the local effective stress. The influence of the smallest precipitates on the creep behavior has been enlightened: they induce narrow channels which act as obstacle for the movement of the dislocations. In the case of the narrowest channel, the deformation can operate by the propagation of Shockley dislocations or else, by the only propagation of the leading partial resulting from the partial dislocation decorrelation. The occurrence of the observed micromechanisms has been quantitatively analyzed using a nodal dislocation dynamics simulation.

Introduction

The polycrystalline NR3 Ni-based superalloy was designed to be used as turbine disk material in aircraft gas turbine engines and exhibits an attractive balance of tensile, fatigue and creep properties [1]. This alloy processed by the powder metallurgy route contains a bimodal precipitation of γ'-$Ni_3(Al, Ti)$ particles embedded in a γ fcc Ni-based solid solution. In a previous study, the influence of the tertiary precipitates on the creep behaviour has been enlightened [2]. In order to provide a thorough understanding of the tertiary precipitates role in the deformation micromechanisms, transmission electron microscope (TEM) *post mortem* observations as well as *in situ* straining experiments on crept samples have been carried out. Different dislocation propagation modes have been pointed out, depending on the local microstructure and on the local effective stress: bypassing or shearing by perfect or partial dislocations. We focused on the mechanisms associated with partial dislocations as they correspond to a localization of plasticity due to narrow γ channels. Dissociated dislocations constrained to move through channels present different types of behaviour. Two different mechanisms involving partial dislocations have been studied in previous papers: the dislocations have been precisely characterized and the local stress corresponding to the observed dislocation configurations have been evaluated [3, 4]. This paper is aimed to give a more general analysis of the condition for each mechanism to occur using a combination of dislocation dynamics simulations, analytical calculations and experimental observations.

Material and experimental details

The NR3 alloy is a polycrystalline superalloy developed at ONERA for high temperature disk applications (ONERA-SNECMA patent). The chemical composition is given Table 1.

Table 1. Chemical composition of the NR3 alloy (wt. %)

Ni	Co	Cr	Ti	Al	Mo	Hf	Zr	C	B
60.69	*14.64*	*11.82*	*5.5*	*3.65*	*3.28*	*0.33*	*0.052*	*0,024*	*0,013*

It was processed by Tecphy and Snecma using the powder metallurgy route. All the thermomechanical operations were conducted below 1205°C which is the γ'-solvus temperature. Then, a supersolvus solution treatment for 2 hours at 1210°C, followed by cooling at 100°C min^{-1}, was used. Primary precipitates, mainly located at the grain boundaries were dissolved by this supersolvus treatment. Subsequently, the following standard heat treatment sequences were used to obtain a bimodal distribution of secondary and tertiary γ' precipitates within the grains (γ' volume fraction around 50%).

TEM experiments have been performed on a JEOL 2010 with an operating voltage of 200kV. The observations have been carried out on NR3 specimens previously creep-strained at 700°C under 500 MPa and 650 MPa with an interrupted creep strain of about 0.2%. The samples were cut normally to the tensile axis from crept specimens.

TEM observations

Microstructure characterization. The microstructure has been investigated in detail: the size, the volume fraction and the γ-channel widths have been determined [5]. An illustration of the microstructure is presented Fig. 1. It consists of a bimodal distribution of secondary and tertiary γ'-precipitates with a mean size of 200 nm and 30 nm respectively. The volume fraction of the tertiary precipitates has been found to be around 3 %. More than 150 measurements of channel widths have been carried out to obtain a good statistic. We have used the most probable width as the pertinent value. The results give a mean value around 25 ± 2 nm.

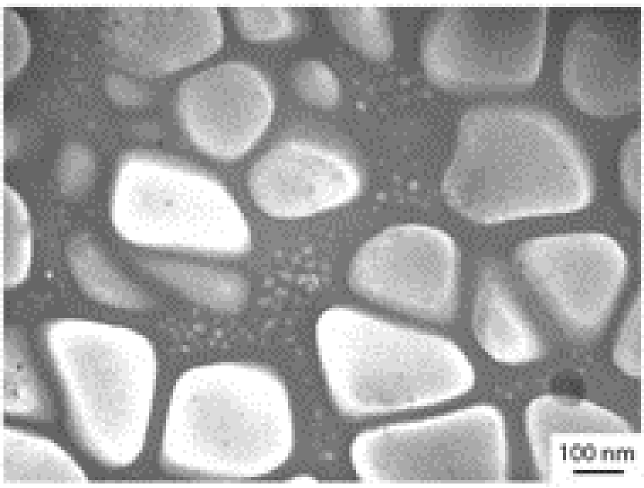
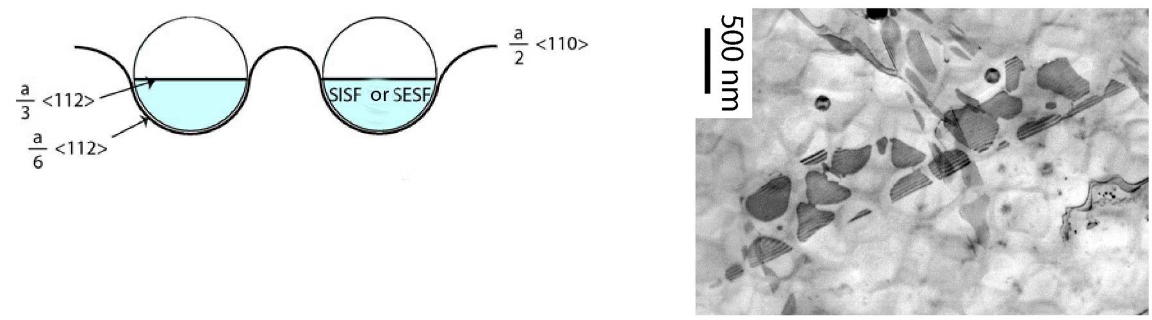


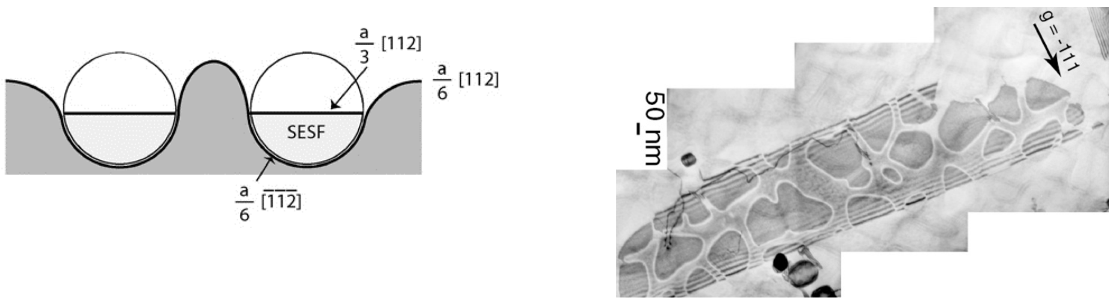
Figure 1. TEM micrograph of the investigated NR3 γ/γ' superalloy.

Deformation micromechanisms. Different micromechanisms have been observed depending on the location within the sample because of different local effective stresses and slightly different microstructures. When a perfect a/2<110> dislocation meets a γ/γ' interface and is unable to cross

it, the dislocation must bend to enter a γ channel, and by-passes the γ’ precipitates, by creating loops around them. This mechanism has been first proposed by Orowan and is a classical one in structural hardening alloys [6]. Another way for the deformation to occur is the propagation of partial dislocations of a/6<112> type resulting from perfect a/2<110> dislocations. Then, other deformation micromechanisms are induced:
i) the “Condat and Décamps” mechanism (Fig. 2a) [7 – 8],
ii) the “Décamps and Raujol” mechanism (Fig. 2b) [3],
iii) the decorrelated movement (Fig. 2c) [4].



a)



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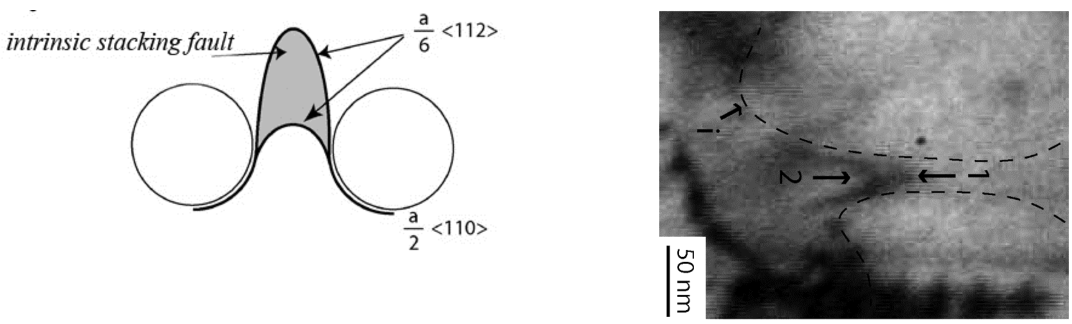

c)

Figure 2. Schematic representation and experimental observations of the different micromechanisms involving partial dislocations; post mortem observations of the *a)* “Condat and Décamps” mechanism and *b)* “Décamps and Raujol” mechanism; *c)* Decorrelation process observed during a TEM in situ straining experiment.

All these mechanisms have been precisely analysed in the literature. The “Condat and Décamps” mechanism results from the motion of a perfect dislocation in the γ phase which dissociates into partials in the γ’ phase. Then, after dislocation motion, secondary as well as tertiary precipitates are surrounded by a partial dislocation and are faulted. The “Décamps and Raujol” mechanism results from shearing of both the matrix and the precipitates by a partial dislocation, the γ matrix and the precipitates being therefore faulted. It has been shown that this process is initiated by a decorrelation process. This uncoupled motion of partial dislocations has been enlightened in this material and exists also in other polycrystalline Ni-based superalloys as well as in monocrystalline Ni-based superalloys [4, 9]. It is a matter of importance as it is at the origin of a frequent shearing process. Many evidences of this phenomenon have been found within *post mortem* samples, as well as during *in situ* straining experiments. From a microstructural point of view, the decorrelation and the Décamps and Raujol mechanisms are directly related to the finest precipitation, that is, to the narrowest channels. This paper is therefore aimed to focus on this decorrelation mechanism.

In order to analyse the conditions for a mechanism to occur, the corresponding necessary stress levels have to be determined. It is clear that they depend on the following parameters: *i)* the characteristics of the alloy (in particular the channel width, the γ' phase volume fraction, the γ' precipitate size, and the γ/γ' interface strength), *ii*) the Burgers vector of the dislocation involved and *iii)* the energy of the fault created during the process. Then, the necessary stress can be compared with the local applied stress. If it is lower than the applied stress, then the associated mechanism is favoured.

Dislocation dynamics simulation and analytical calculation

In order to give a quantitative analysis of the correlation between local effective stress and decorrelated movement as exhaustive as possible, we have developed analytical calculation and dislocation dynamics simulation.

Decorrelation of the partial dislocation movement occurs when the effective stress acting on the perfect dislocation does not allow it to propagate as a whole, in the matrix channel, while this propagation is possible for the leading partial dislocation. When a dislocation is pushed towards the entrance of a channel between two obstacles, it must bend to enter the channel. The necessary stress to bend a dislocation is proportional to the rigidity of the dislocation. This can be defined by the line tension, which is proportional to μb^2 in a first approximation [10]. Therefore the necessary stress to bend a dislocation decreases with the modulus of b so that a partial dislocation should enter a channel more easily than a perfect one. To quantify this, it is necessary to calculate the threshold stress acting on the perfect dislocation and on each one of the partial dislocations. In fact, the behavior of a dislocation in such confining conditions is difficult to model precisely for three main reasons: (i) the local properties of a dislocation change with the orientation of its line, and in particular its flexibility; (ii) each segment of the dislocation interacts with every other segments of dislocations, including itself; (iii) the dislocation strongly interacts with the local environment during its motion and its expansion is constrained by the shape of the channels. In the case of partial dislocations, an additional level of complexity results in this splitting into partial dislocations bounding a stacking fault.

We have first defined the magnitude of the τ_L and τ_r effective shear stresses acting respectively on the leading and the trailing partial bordering a stacking fault with energy γ_{SF}, at angle α from the channel direction, assuming isotropic elasticity, and neglecting self-interaction as well as interaction between the partial dislocations. They are given by the following equations (Eq. 1 and Eq. 2):

$$\tau_L(\alpha) = \left(\frac{2E_s(\theta_L)}{Hb_L} + \frac{\gamma_{SF}}{b_L} \right) \frac{1}{\cos(\alpha + \theta_L)} \qquad (1)$$

$$\tau_T(\alpha) = \left(\frac{2E_s(\theta_T)}{Hb_T} - \frac{\gamma_{SF}}{b_T} \right) \frac{1}{\cos(\alpha - \theta_T)} \qquad (2)$$

where H is the width of the channel, φ is the angle between the effective shear stress $\vec{\tau}$ and the Burgers vector $\vec{b}$, θ the angle between the orientation of the channel and $\vec{b}$, and α the angle between the orientation of the channel and the effective shear stress $\vec{\tau}$ (cf. Fig.3).

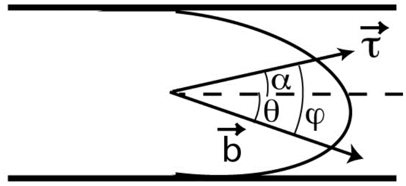

Figure 3. Schematic shape of a dislocation gliding through a channel. $\vec{\tau}$ is the effective shear stress and $\vec{b}$ its Burgers vector.

Using Eq. 1 and Eq. 2, it is clear that the two partials propagate differently through the channel and with asymmetrical shapes. Then, in order to go further as this analytical calculation neglects the interplay between dislocations flexibility, long-range interactions of dislocation segments, applied stress and width and orientation of the channel, we have developed a discrete dislocation dynamics simulation that includes all these different effects as well as dissociation. The dislocations are represented by a set of nodes connected by small segments. This allows a better description of the smallest changes in the orientation of the dislocation, thus preserves the slightest influence of the line tension. The simulation follows the now classic scheme of calculating the force at a point of the dislocation from the total applied stress using the Peach-Koehler formulation $F = \left(\overline{\overline{\sigma}}.\vec{n}\right).\vec{b}$ where F is the modulus of the force acting perpendicular to a segment of a dislocation in a plane defined by $\vec{n}$ and $\overline{\overline{\sigma}}$ is the applied stress tensor [11]. The simulations were conducted for a dissociated dislocation moving in a channel surrounded by impenetrable obstacles. In order to validate the simulation, we have compared our results with experimental observations. As illustrated Fig. 4, an excellent agreement is obtained between the decorrelated movement observed Fig. 2c and the corresponding simulation.

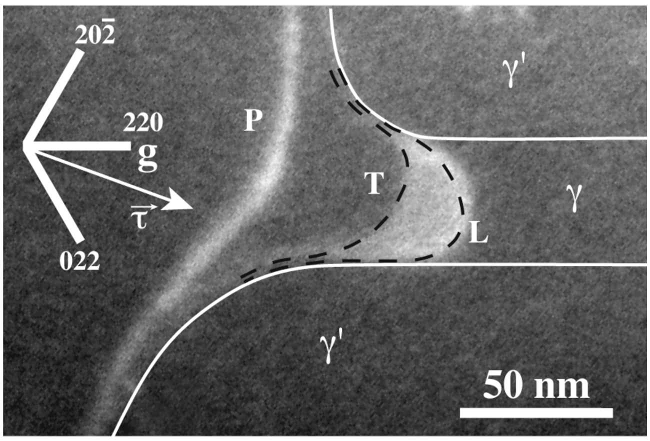

Figure 4. Comparison between experimental observed decorrelation movement and the positions of the partial dislocations (in dotted line) as obtained using dislocation dynamics simulation. The leading dislocation was moving in the $(1\bar{1}1)$ plane towards a 40 nm wide channel parallel to [110] and delimited by two impenetrable γ' precipitates. The parameters used are those of the γ-phase of a Ni-based superalloy : μ = 58.6 GPa [12], ν = 1/3 and the fault energy is γ_{SF} = 0.025 J/m^2 [13]. P stands for perfect dislocation, while L and T refer to leading and trailing partial respectively.

Repeating numerous dislocation dynamics simulations, using different stress magnitudes and orientations, for a fixed channel width, *three types of behavior* have been evidenced: *i)* none partial dislocation goes through the channel, *ii)* only one partial goes through, *iii)* the two partial dislocations go through. All these situations are synthesized in a previous paper [14]. The remarkable result is that the deformation may occur using partial dislocation propagation at a stress level lower than expected for a perfect one (up to 30% less) resulting in microplasticity. Such phenomenon has to be taken into account for a precise description of the macroscopic behavior when the material experiences low stress level during a long period as it is often the case in creep regime. To conclude, it appears then essential to include partial dislocations bordering a stacking fault in any mechanical modeling when impenetrable obstacles confine plasticity.

Summary

Amongst the numerous dislocation mechanisms operating in Ni-based superalloys, the elementary deformation mechanisms associated with the entering of a dissociated dislocation into a γ narrow channel have been quantitatively analyzed using a combination of dislocation dynamics simulation, analytical calculation, and TEM observations. Many evidences of individual partial dislocation propagation have been pointed out. The threshold stress associated with the propagation of each partial through a channel has been established. In addition, dislocation dynamics simulation has shown the large occurrence for this mechanism, as observed by TEM. As the movement of partial dislocation can induce microplasticity, it is an important mechanism to be included in mechanical properties modeling because it can play a significant role during low stress creep regime.

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