A Strain Rate Sensitive Formulation to Account for the Effect of γ' Rafting on the High Temperature Mechanical Properties of Ni-Based Single Crystal Superalloys

Jean-Briac le Graverend, Jonathan Cormier, Serge Kruch, Franck Gallerneau and José Mendez

Abstract The ***Polystar*** model was recently developed to fulfill the effects of possible fast microstructure evolutions occurring upon high temperature non-isothermal loadings. New internal variables were introduced in a crystal plasticity framework to take into account microstructure evolutions such as γ' dissolution/precipitation and dislocation recovery processes, and their effects on the creep behavior and creep life. Nevertheless, this model does not take into account one of the main microstructural evolutions occurring specifically at high temperature, the γ' directional coarsening. Fedelich and Tinga have already proposed models respectively based on a modification of the kinematic hardening and on the level of the von Mises stress. Nevertheless, if the Fedelich's model is implicitly strain rate sensitive, improvements have to be performed for strain controlled tests under fast conditions for which such a model may overestimates the γ channel width evolutions. A new formulation has been proposed to explicitly account for such a strain rate sensitivity and was successfully implemented in the ***Polystar*** model. The effect

J.-B. le Graverend (✉) · S. Kruch · F. Gallerneau
Onera, 29 avenue de la Division Leclerc, BP 72, 92322 Châtillon, France
e-mail: jean-briac.le_graverend@onera.fr

S. Kruch
e-mail: serger.kruch@onera.fr

F. Gallerneau
e-mail: franck.gallerneau@onera.fr

J.-B. le Graverend · J. Cormier · J. Mendez
Institut P', CNRS-ENSMA-Université de Poitiers, UPR CNRS 3346, ENSMA-Téléport 2, 1 avenue Clément Ader, BP 40109, 86961 Futuroscope Chasseneuil Cedex, France

J. Cormier
e-mail: jonathan.cormier@ensma.fr

J. Mendez
e-mail: jose.mendez@ensma.fr

H. Altenbach and S. Kruch (eds.), *Advanced Materials Modelling for Structures*, Advanced Structured Materials 19, DOI: 10.1007/978-3-642-35167-9_18,

of γ' rafting on the mechanical behavior is well reproduced for both cyclic and monotonic tension tests.

1 Introduction

Monocrystalline nickel base superalloys are widely used in the hottest parts of aero-engines or industrial gas turbines [1]. Blades made of these alloys operate for thousands of hours at temperatures as high as 1373 K (1100 °C) [2]. These alloys are chosen for their superior mechanical performances at high temperatures, in particular their creep resistance for uncooled components such as high pressure turbine blades of turboshaft engines for helicopters or small industrial gas turbines. These interesting properties result from the precipitation of a high volume fraction (close to 70 %) of the long-range ordered $L1_2$ γ' phase which appears as cubes coherently embedded in a face-centered cubic (fcc) solid solution γ matrix.

The recent development of "microstructure sensitive models" (i.e. in which internal variables representing microstructure are added) has been motivated by need to obtain a better predictivity of the mechanical behavior under conditions where microstructure is likely to evolve during the thermomechanical loading. Indeed, under such conditions, classical constitutive modelling approaches where temperature dependence is only taken into account by the temperature dependence of the material's parameters fails to predict transient mechanical responses of the alloy during thermomechanical loading [3]. For example, such a modelling approach is undertaken to account for the impact of the γ' morphology evolution under directional coarsening conditions on the mechanical properties of Ni-based single crystal superalloys [4, 5]. Indeed, when a single crystal superalloy has a negative γ/γ' misfit (coherency stress due to the difference between the lattice parameters of the γ phase and the γ' phase), a directional coarsening of the γ' precipitates occurs perpendicularly to the applied stress axis (see Fig. 1). This morphological evolution, more widely known under the "γ' rafting" denomination, usually takes place during the primary creep stage when the γ' phase has entirely coalesced and the γ channels become wider along the applied stress axis (see Fig. 1) [6–8].

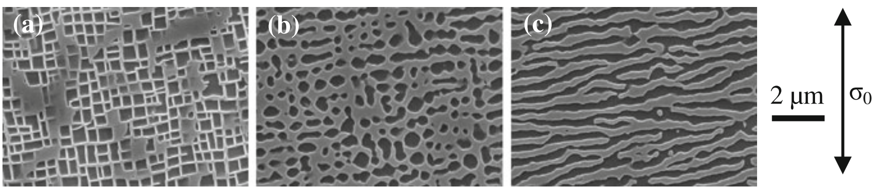

Fig. 1 γ' rafting during a creep test at 1050 °C/160 MPa: γ/γ' microstructure at the beginning of the experiment (**a**), after 4.7 h (during primary creep stage) (**b**) and after 9.4 h (beginning of secondary creep stage) (**c**). Note that the γ' phase appear in *dark*

In this article, a set of constitutive equations that is able to account for the rafting kinetics under isothermal and non-isothermal loading without requiring a computationally intensive microstructural analysis will be detailed. The ***Polystar*** model recently developed under a crystal plasticity framework was used to implement new evolution laws to account for a strain rate sensitivity of the γ' rafting [9].

2 Model Presentation

The ***Polystar*** model has been developed under a crystal viscoplasticity framework using the Méric & Cailletaud model as a basis [10]. It only considers the activity of octahedral slip systems since no experimental evidences of cube slip support the use of such systems [11]. A full description of the ***Polystar*** model is available elsewhere [9]. Only the equations devoted to account for the impact of γ' rafting will be discussed in the present article.

In this model first devoted to the creep behavior modelling, only non-linear isotropic hardening was considered for the evolution of internal stresses. The impact of γ' microstructural evolutions was taken into account using an Orowan stress which was introduced in the isotropic hardening using the following formulation:

$$r^s = \tau_0^s + b \times (Q + Q^*) \times \sum_j h_{sj} \rho^j + \sqrt{\frac{2}{3}} \frac{Gb}{w_{001}} \tag{1}$$

The Orowan stress is the last term of Eq. (1) while the first and the second terms of this equation represent respectively the initial critical resolved shear stress on each octahedral slip systems and the dislocation hardening through the isotropic state variable ρ^s and cross hardening by means of the interaction matrix [h]. Q is a temperature dependent material parameter which depends on the temperature and which corresponds to a steady-state dislocation hardening. Q^* is a transient hardening which is time and temperature dependent through the evolution of an associated internal variable a^* [9].

The initial expression of the γ-channel width along a [001] direction (w_{001}) was the following one:

$$w_{001} = \frac{a_0}{\delta} \times (f_l^{ml} - dtp \times f_s) \tag{2}$$

f_l and f_s represent respectively the volume fractions of large and hyperfine γ' precipitates of a bimodal distribution of γ' particles. dtp, a_0 and δ are model parameters.

It was decided to modify this equation to take into account the γ' microstructure degradation occurring at high temperature. This microstructure degradation basically consists in a homothetic particle growth due to Ostwald ripening ($w_{isotropic}$ in Eq. (3))

and in a directional coarsening (i.e. γ' rafting, see e.g. Fig. 1) under the action of mechanical applied stress ($w_{mechanic}$ in Eq. (3)).

Thus, a new expression of the γ-channel width evolution is proposed which both satisfy γ channels widening under pure isothermal conditions and during non-isothermal solicitations:

$$w_{001} = w_0 \times w_{thermic} \times (1 + w_{mechanic} + w_{isotropic}) \tag{3}$$

$w_{thermic}$ keeps the formulation proposed by Cormier and Cailletaud, as defined in their model [9]:

$$w_{thermic} = f_l^{ml} - dtp \times f_s \tag{4}$$

Moreover, the yield criterion was modified to take into account the kinematic hardening:

$$f = \left|\tau^s\right| - r^s \rightarrow f = \left|\tau^s - x^s\right| - r^s \tag{5}$$

2.1 Homothetic Growth

The driving force for isotropic coarsening is the reduction of the internal γ/γ' interfacial energy. For this reason, the $w_{\text{isotropic}}$ variable will only be time and temperature dependent and not deformation/stress state dependent.

Contrary to what has been proposed by Fedelich et al. [5], it was decided to use a cube root with a temperature dependent model parameter:

$$w_{isotropic} = \sqrt[3]{1 + \chi_0 e^{\frac{-U_t}{RT}} t} \tag{6}$$

In this equation, T is the temperature in Kelvin, U_t an activation energy, R the perfect gas constant and χ_0 a model parameter independent of the temperature.

Indeed, according to the Lifschitz-Slyozov-Walter (LSW) theory, particles coarsening controlled by diffusion processes is cube root dependent on time when the precipitate volume fraction is small [12]. This theory was developed for a binary system and for spherical particles which is not the case for single crystal superalloy. However, Ardell and Nicholson [13] have shown that the assumption of a diffusion-controlled growth stayed available in Ni-based single crystal superalloys. Moreover, Brailsford and Wynblatt [14] have shown that this type of particle growth led to an exponent equal to 3 in the LSW theory.

2.2 Directional Coarsening

Matan et al. have shown that a creep strain threshold was necessary to be overcome so that the γ' rafting process become significant and can proceeds, still in absence of any applied stress [15]. This threshold is equal to 0.10 ± 0.03 % at 950 °C for CMSX-4® alloy. Indeed, as Embury et al. [16] have shown, dislocations enhance the diffusion processes by pipe-line diffusion. Thus, once a given dislocation density at the γ/γ' interfaces is reached (corresponding to the relaxation of coherency stresses), the γ' rafting process occurs.

For this reason, it was chosen to develop a set of constitutive equations to account for γ' rafting dependence on the accumulated viscoplastic strain. Indeed, using the accumulated viscoplastic strain (v) as the internal variable driving the γ' rafting in Eq. (7), rafting will continue at high temperature even if the external load is removed.

Moreover, in case of tests with large viscoplastic strain amplitudes or fast thermomechanical solicitations, it was necessary to consider a strain rate dependence to be able to reproduce all types of test (i.e. cyclic loading. stress relaxation, tension tests, etc.). w_{mechanic} was hence given the following expression depending on the new internal variable (ξ) accounting for the strain rate sensitivity (Eq. (8)).

$$w_{mechanic} = \frac{K_0 \times \left(1 - e^{-\frac{t}{\tau_{diffusion}}}\right) \times \sqrt[3]{v}}{1 + \sinh^{-1}(\xi \times v_0)} \tag{7}$$

$$\dot{\xi} = \left(\frac{\dot{v}^2}{\xi_0} - \xi\right) \times \dot{v} - \left(\frac{\xi}{M}\right)^m \tag{8}$$

In these equations, M, m, ξ_0, v_0 and K_0 are temperature dependent model parameters.

The first term of Eq. (8) allows to smooth evolutions of $w_{mechanic}$ during fast strain controlled tests ($\dot{\varepsilon} \geq 10^{-4}\,\mathrm{s}^{-1}$): the faster the test is, the higher ξ is, leading to a decrease of $w_{mechanic}$. The second term of Eq. (8) allows obtaining a recovery effect in case of mechanical tests for which a large strain rate range can be encountered.

$$\tau_{diffusion} = \frac{d^2}{2 \times D_{Al}^{\gamma'}(T)} \tag{9}$$

For the specific time of diffusion (Eq. (9)), it was chosen to consider the diffusion of aluminium in the γ' phase since it was observed that the rate limiting factor of γ' rafting is the diffusion of γ' elements in the γ' phase [17]. Hence, $D_{Al}^{\gamma'}$ is the diffusion coefficient of aluminium in the γ' phase (unit in m^2/s) and d is the diffusion mean free path for diffusion (unit in m) (see [18] and [19] for more details).

3 Results

3.1 Channel Width Calibrations

The parameters involved in the γ channel width evolutions given through Eqs. (6)–(9) were calibrated using interrupted creep tests and subsequent image analyses for several conditions of stress and temperature. Two examples of these evolutions at 1050 °C under 140 MPa and 1200 °C under 67 MPa are given in Fig. 2 for MC2 alloy.

It can be observed a rather good representation of the γ channel width evolution, within the scatter of the experimental results. Thus, the new formulation proposed to account for the γ' microstructure degradation through the increase in the γ channel width has been calibrated using creep tests under different temperature/stress conditions and is subsequently used to account for the impact of γ' coarsening on high temperature tensile or LCF properties.

3.2 Mechanical Behavior

The aim of the strain rate formulation is to obtain an evolution of γ channel width which allows to account for the impact of the (long term) γ' degradation on the mechanical properties. Indeed, the γ channel width does not evolve during fast tests and a minimum time (or plastic deformation) is required to trigger the γ' rafting. Thus, the predictivity of the modified version of the ***Polystar*** model including kinematic hardening and the microstructure degradation equations (Eq. (6)–(9)) was assessed using different mechanical tests.

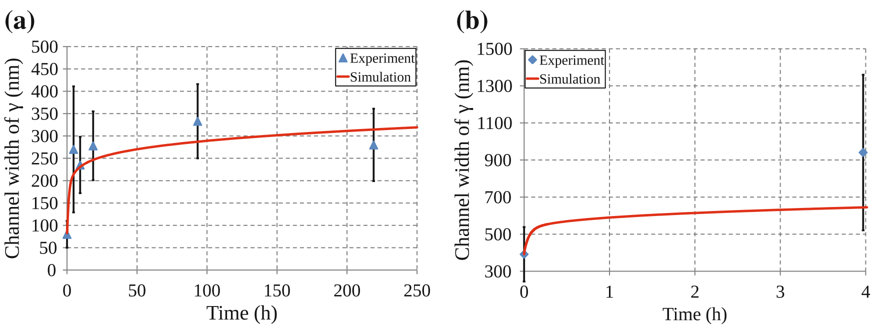

Fig. 2 Experimental evolutions of the γ channel width during creep tests at 1050 °C/160 MPa (**a**) and at 1200 °C/67 MPa (**b**) compared with the ***Polystar*** calibrations

3.2.1 Creep Tests

To get a first estimation of the potential benefits of this modified version of the **_Polystar_** model, three isothermal creep tests were studied (see Fig. 3).

To only consider the impact of the microstructure degradation on the mechanical behavior (i.e. primary and secondary creep stages), the damage equations of the **_Polystar_** model were inactivated. It can be observed in Fig. 3 that the longer the creep test, the better the predictability of the modified **_Polystar_** model. Indeed, it is observed a better prediction of the secondary creep strain rate for longer creep tests where the γ' rafting is the most pronounced.

Moreover, the strain rate formulation used for the γ channel width evolution gives an evolution of the Orowan stress in good agreement with Fedelich's results [5] (see Fig. 4. However, the plastic strain threshold observed by Matan et al. [18] equal to 0.1 ± 0.03 % necessary to trigger γ' rafting (and hence, the Orowan stress decrease) is not captured by our model, as for the Fedelich one.

The new formulation of the **_Polystar_** model was also validated using complex non-isothermal experiments. As an example, the predictivity of the model was assessed using a non-isothermal creep test including first an isothermal part at 1050 °C/120 MPa for 24 h and then a thermal cycling under 120 MPa which consists in 15 min/1050 °C–1 min/1100 °C–15 min/1050 °C–1 min/1150 °C repeated four

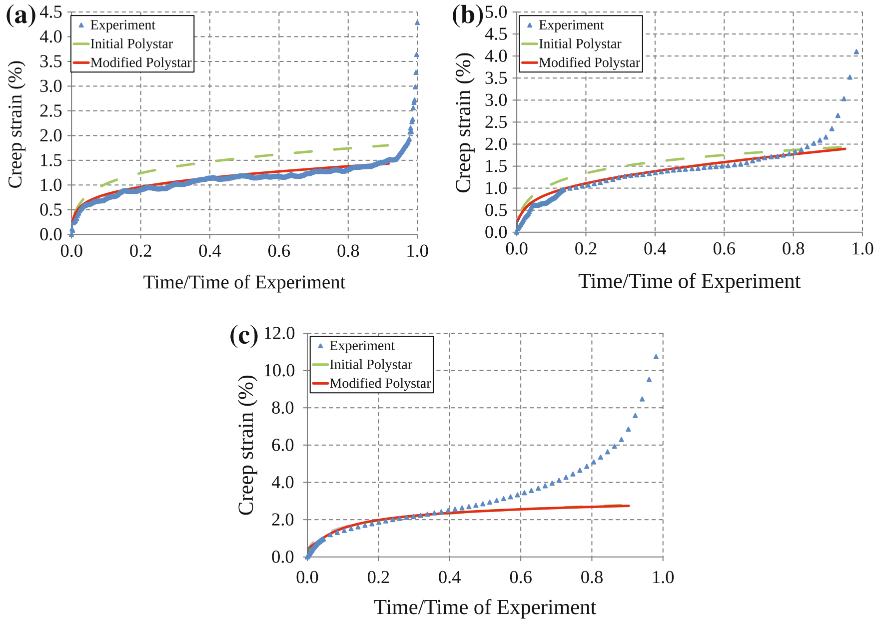

Fig. 3 Comparison between experiments and simulations for creep tests at 1050 °C/160 MPa (**a**), 1050 °C/180 MPa (**b**) and 1050 °C/230 MPa (**c**)

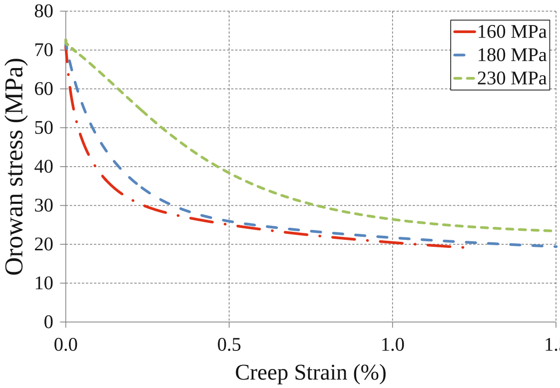

Fig. 4 Evolution of the Orowan stress as a function of creep strain for three different applied stresses at 1050 °C

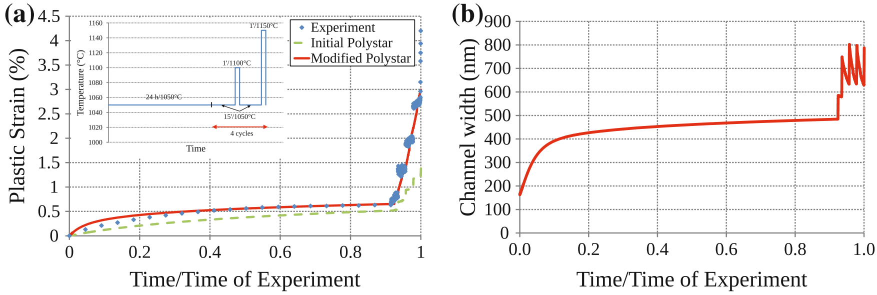

Fig. 5 Comparison between simulations and experiment during a non-isothermal creep test whose reference level is 1050 °C/120 MPa. The thermal and stress loading appears as insert in **a** while **b** shows the numerical evolution of the γ channel width during test

times (see Fig. 5). The modified ***Polystar*** model gives a better simulation especially for strain jumps during the non-isothermal section of the test (Fig. 5a). Indeed, it was evidenced that during such kind of non-isothermal experiments, the γ' rafting is very detrimental to the creep strain rate and life [20]. Such an impact is well captured by the present version of the model.

3.2.2 Cyclic Tests

Figure 6 shows the comparison between the experiments and simulations performed with the original and modified version of the model. Even if the stress levels do not corresponds perfectly with the experimental ones, the numerical evolutions of γ channel width are in good agreement with what has been observed experimentally. Indeed, as shown by Gaubert [21] for the AM1 alloy at 950 °C, a slow cyclic test ($d\varepsilon/dt \leq 10^{-5}\,s^{-1}$) with a fully reversed strain cycling leads to microstructural

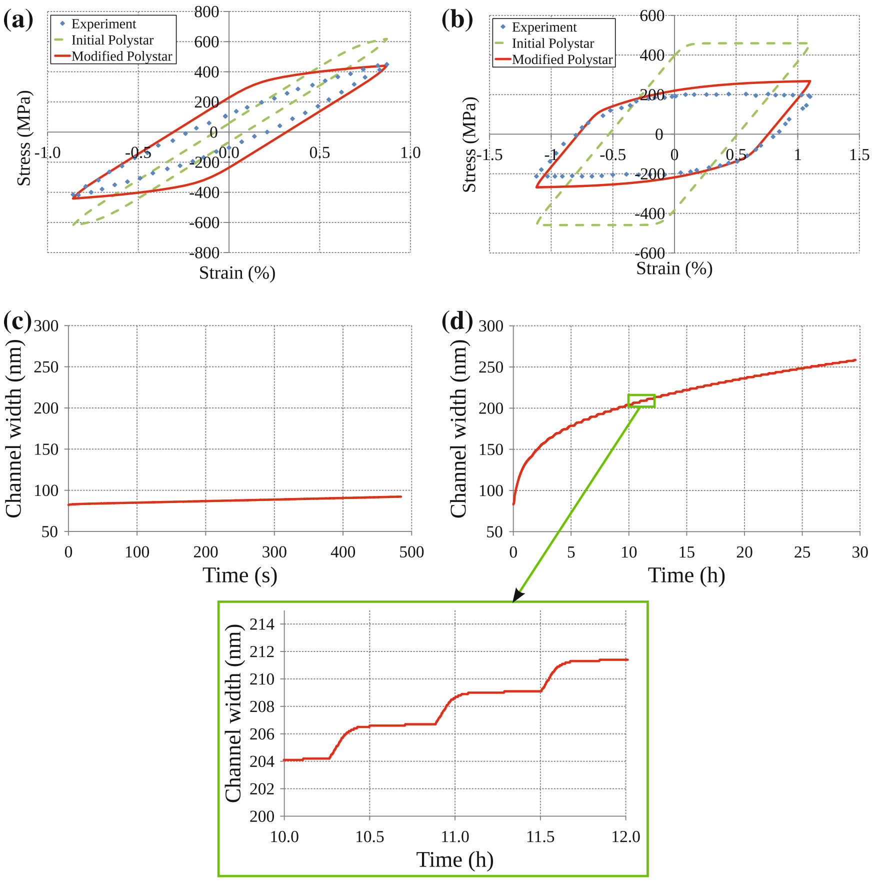

Fig. 6 Comparison between experiments and simulations for two LCF conditions using different strain rates and strain amplitudes at 1050 °C: 14th cycles at $10^{-3}\,s^{-1}$ (**a**) and 24th cycles at $10^{-5}\,s^{-1}$ (**b**). **c** and **d** represent respectively the numerical evolution of γ channel width presented in **a** and **b**

evolutions characterized by a 45° orientation of the γ' rafting with respects to the tension/compression axis. Hence, for a same number of LCF cycles, the γ channel width will be smaller in case of a fast mechanical cycling test compared to a slow cycling one.

3.2.3 Tensile Tests

Two strain rates were also investigated for tensile tests (10^{-3} and $10^{-5}\,s^{-1}$) to analyze the model sensitivity to the strain rate (see Fig. 7).

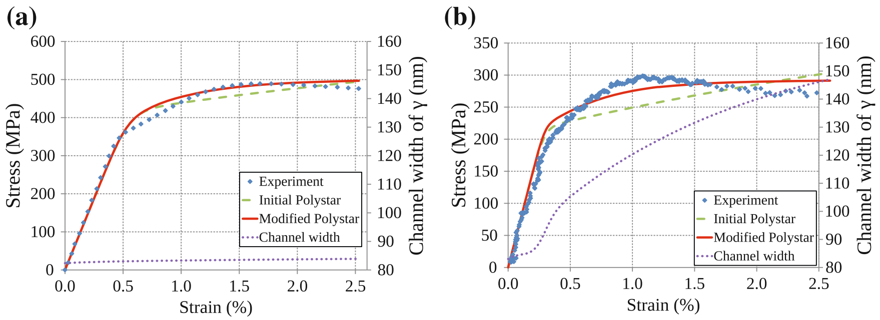

Fig. 7 Comparison between experiments and simulations during tensile tests at 1050 °C:10^{-3} s^{-1} (**a**) and $10^{-5}\,s^{-1}$ (**b**). *Purple curves* represent the evolution of γ channel width during simulations

Modifications bring to the model slightly improve the modelling of the tensile behavior.

Moreover, a comparison between experiment and simulations for a tensile test under variable strain rate shows that the modified version of the ***Polystar*** model provides a better description of the viscoplastic part. When the strain rate decreases from 10^{-3} to $10^{-5}\,s^{-1}$, the experimental decrease of stress is equal to 145 MPa whereas the initial ***Polystar*** and the modified ***Polystar*** gives respectively 195 and 175 MPa.

4 Conclusion

The strain rate sensitive formulation developed to account for the effect of γ' rafting on the high-temperature mechanical properties of Ni-based single crystal superalloys gives results in good agreement with experiments over a wide range of strain rate: from 10^{-3} to $10^{-8}\,s^{-1}$.

The consideration of microstructural evolutions was successful in the prediction of the non-isothermal creep behavior after a γ' microstructure degradation.

Thus, this new formulation is an advanced modelling tool for the prediction of both microstructural evolutions at high-temperature for Ni-based single crystal superalloys and their impact on the mechanical properties.

Acknowledgments The authors are particularly grateful to Turbomeca-SAFRAN group for providing the material and to the DPAC (Direction des Programmes Aéronautiques et de la Coopération) for its financial support. This work is conducted under a French program involving Snecma-SAFRAN group, Turbomeca-SAFRAN group, ONERA, CNRS laboratories (Mines Paris Tech, Institut P'-ENSMA, LMT-Cachan, LMS-X, CIRIMAT-ENSIACET) and CEAT.

J.-B. le Graverend is also grateful to D. Pacou, V. Bonnand and R. Degeilh for stimulating discussions.

References

1. Caron, P., Khan, T.: Mater. Sci. Eng. **61**, 173–184 (1983)
2. Reed, R.C.: The Superalloys: Fundamentals and Applications. Cambridge University Press, Cambridge (2006)
3. Cailletaud, G.: Doctoral Thesis. Université Pierre et Marie Curie, France (1979)
4. Tinga, T., Brekelmans, W.A.M., Geers, M.G.D.: Comp. Mater. Sci. **47**, 471–481 (2009)
5. Fedelich, B., Künecke, G., Epishin, A., Link, T., Portella, P.: Mater. Sci. Eng. A **510–511**, 273–277 (2009)
6. Henderson, P., Berglin, L., Jansson, C.: Scripta Mater. **40**, 229–234 (1999)
7. Sass, V., Glatzel, U., Feller-Kniepmeier, M.: Acta Mater. **44**, 1967–1977 (1996)
8. Shui, J., Tian, S., Jao, T., Hu, Z.: Mat. Sci. Eng. A **418**, 229–235 (2006)
9. Cormier, J., Cailletaud, G.: Mater. Sci. Eng. A **527**, 6300–6312 (2010)
10. Méric, L., Poubanne, P., Cailletaud, G.: J. Eng. Mater. Technol. **113**, 162–171 (1991)
11. Vattré, A., Devincre, B., Roos, A.: Acta Mater. **58**, 1938–1951 (2010)
12. Lifshitz, I.M., Slyozov, V.V.: J. Phys. Chem. Solids **19**, 35–50 (1961)
13. Ardell, A.J., Nicholson, R.B.: J. Phys. Chem. Solids **27**, 1793–1804 (1966)
14. Brailsford, A.D., Wynblatt, P.: Acta Metall. **27**, 489–497 (1979)
15. Matan, N., Cox, D.C., Rae, C.M.F., Reed, R.C.: Acta Mater. **47**, 2031–2045 (1999)
16. Embury, J.D., Deschamps, A., Brechet, Y.: Scripta Mater. **49**, 927–932 (2003)
17. Reed, R.C., Cox, D.C., Rae, C.M.F.: Mater. Sci. Tech. **23**, 893–902 (2007)
18. Matan, N., Winand, H.M.A., Carter, P., Karunaratne, M., Bogdanoff, P.D., Reed, R.C.: Acta. Mater. **46**, 4587–4600 (1998)
19. le Graverend, J.-B., Cormier, J., Gallerneau, F., Paulmier, P.: Adv. Mater. Res. **278**, 31–36 (2011)
20. Cormier, J., Jouiad, M., Hamon, F., Villechaise, P., Milhet, X.: Phil. Mag. Lett. **90**, 611–620 (2010)
21. Gaubert, A.: Ph.D. Thesis. Mines Paris-Tech., France (2009)