

SEGREGATION-ASSISTED PLASTICITY IN NI-BASED SUPERALLOYS: A COUPLED EXPERIMENTAL AND MODELLING STUDY

D. Barba¹, D. García-González¹, E. Alabort², J. Moverare³, R.C. Reed^{1,2}, A. Jérusalem^{1,*}

¹Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ, United Kingdom

²Department of Material Science, University of Oxford, Parks Road, Oxford, OX1 3PH, United Kingdom

³Division of Engineering Materials, Department of Management and Engineering, Linköping University, SE-58183 Linköping, Sweden

Key Words: *Crystal plasticity, diffusion, multi-scale, multi-physics*

A novel plastic deformation mechanism has been reported recently in Ni-based superalloys in the mid-temperatures range (700-900°C) [1,2]. This deformation mechanism, microtwinning, involves diffusional processes coupled with plastic shearing in a phase transformation fashion [2]. The range of temperatures at which microtwinning occurs is of increasing interest among metallurgists and engineers as aircraft turbine parts are now operating in this regime. Chemical fluctuations around the twins' tips are believed to play an important role in the kinetics of the process [1,2]. The coupled diffusive-displacive nature [1,2] of this mechanism makes microtwinning a thermally-activated phenomenon. The precise details of this mechanism are not yet well understood [2] and accurate continuum models have not yet been proposed until now [3].

In this study, experiments and modelling are coupled together to gain a full understanding of the problem. First, the diffusion processes and chemical changes around the growing microtwins are studied using atom probe tomography and transmission electron microscopy. Second, these observations are used to model the kinetics of the mechanism at the lower scale using diffusion theory. Finally, a thermodynamically consistent continuum framework is developed which links the acquired knowledge from the lower scale to the macroscopic behaviour. The driving forces for the different deformation mechanisms are extracted directly from the first and second Principle of Thermodynamics, thus ensuring the energetic consistency of the model. A multiscale approach is used to relate the influence of the chemical composition at the atomistic scale to the flow rule at the microscale through the free energy function of the system. In turn, the composition is dependent on the deformation rate through the diffusion theory formulated at the lower scale, thus making it a closed problem.

The constitutive model was implemented into a CP-FE code and calibrated against creep experiments of single crystal superalloy MD2 to study the activation of the different plastic mechanisms within single crystal and polycrystalline models. The model predicts with accuracy the high anisotropic behaviour and tension-compression asymmetry of the single crystals for all the studied crystal orientations ($\langle 001 \rangle$, $\langle 011 \rangle$ and $\langle 111 \rangle$) and of the polycrystalline alloy. For the first time, the numerical and experimental results reveal the critical role of the strong directionality of microtwin nucleation on the material asymmetric behaviour and the link between microtwin formation and premature failure. At this scale, the acquired mechanistic knowledge of the microtwinning process allows for a better understanding of the ability of superalloys to withstand the extreme conditions at which some of the most critical aerospace components operate.

REFERENCES

- [1] On the microtwinning mechanism in a single crystal superalloy. D. Barba, E. Alabort, S. Pedrazzini, D.M. Collins, A.J. Wilkinson, P.A.J. Bagot, A. Jérusalem, R.C. Reed. *Acta Materialia* 135:314-329
- [2] Phase transformation strengthening of high-temperature superalloys. T.M. Smith, B.D. Esser, N. Antolin, A. Carlsson, R.E. Williams, A. Wessman, T. Hanlon, H.L. Fraser, W. Windl, D.W. McComb, M.J. Mills, (2016). *Nature Communications*, 7, 13434.
- [3] A thermodynamically consistent model for diffusive strain-induced phase transformations: Application to mid-temperatures creep in Ni-based superalloys. D. Barba, D. Garcia-Gonzalez, E. Alabort, R.C. Reed., A. Jérusalem. *International Journal of Plasticity* (accepted).