A thermodynamically consistent model for diffusive strain-induced phase transformations: Application to mid-temperatures creep in Ni-based superalloys

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Mid-temperatures creep deformation mechanisms are of increasing interest among metallurgists and engineers as aircraft turbine parts are now operative in this temperature range (700-900°C). Microtwinning is emerging as one of the most important plastic deformation phenomena in this regime [1]. During deformation, partial dislocations shear the material in a viscous way accompanied by a diffusion assisted phase transformation [2]. Chemical fluctuations around the twin tip are believed to play an important role in the kinetics of the process [3, 4]. The coupled diffusive-displacive nature [1, 2] of this mechanism makes microtwinning a thermally-activated phenomenon. Unfortunately, the precise details of this mechanism are not yet well understood [3]. In particular, accurate continuum models do not exist as of yet. Moreover, important questions remain concerning the role of segregation of alloying elements along the twins [3, 4, 5, 6].

In this study, the kinetics of the mechanism are first modelled at the lower scale using diffusion theory, motivated by the recent findings of chemical fluctuations linked with the plastic flow [6]. Secondly, a continuum mechanics theory is developed which links the acquired knowledge from the lower scale to the macroscopic behavior. The driving forces for the observed predominant mechanisms within 700-900°C (segregation-assisted shearing) 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 link the influence of the chemical composition at the atomistic scale with the flow rule at the microscale trough the free energy function of the system. In turn, the composition is dependent on the deformation rate through the diffusion theory formulated before, thus making it a closed problem. The material parameters of the model are obtained from the microstructural analysis of single crystal superalloy MD2 specimens after creep testing. The constitutive model has been implemented into a CP-FE code to study the activation of the different plastic mechanisms within single-crystal and polycrystalline models. The model predicts with accuracy the activation and propagation of the twin ledges, both of which observed experimentally. For the first time, the numerical and experimental results reveal the critical role of the strong directionality of microtwin nucleation on the asymmetry behaviour and the link between microtwin formation and premature failure of the material. At this scale, the acquired mechanistic knowledge of the microtwinning process allows for a better understanding of how superalloys withstand the extreme conditions at which some of the most critical aerospace components operate.

[1] L. Kovarik, R.R. Unocic, J. Li, P. Sarosi, C. Shen, Y. Wang, and M.J. Mills. Microtwinning and other shearing mechanisms at intermediate temperatures in Ni-based superalloys. Progess in Materials Sicence, 54:839-873, 2009.
[2] M. Kolbe. The high temperature decrease of the critical resolved shear stress in nickel-base superalloys. Progess in Materials Sicence, A319-321:383{387, 2001.
[3] T.M. Smith, B.D. Esser, N. Antolin, G.B. Viswanathan, T. Hanlon, a. Wessman, D. Mourer, W. Windl, D.W. McComb, and M.J. Mills. Segregation and η phase formation along stacking faults during creep at intermediate temperatures in a Ni-based superalloy. Acta Materialia, 100:19-31, 2015.
[4] M.S. Titus, A. Mottura, G.B. Viswanathan, A. Suzuki, M.J. Mills, and T.M. Pollock. High resolution energy dispersive spectroscopy mapping of planar defects in L12-containing Co-base superalloys. Acta Materialia, 89:423-437, 2015.
[5] G. B. Viswanathan, R. Shi, A. Genc, V. A. Vorontsov, L. Kovarik, C. M. F. Rae, and M. J. Mills. Segregation at stacking faults within the 0 phase of two Ni-base superalloys following intermediate temperature creep. Scripta Materialia, 94:5-8,
2014.
[6] D. Barba, S. Pedrazzini, A. Vilalta-Clemente, A. J. Wilkinson, M. P. Moody, P. A. J. Bagot, A. Jérusalem, R. C. Reed, On the composition of microtwins in a single crystal nickel-based superalloy, Scripta Materialia 127 (2017) 37–40.