AFRL-AFOSR-UK-TR-2023-0042

Fundamentals of Deformation Mechanisms in Polycrystalline Superalloys

Roger Reed
THE UNIVERSITY OF OXFORD
UNIVERSITY OFFICES
OXFORD, ,
GB

02/28/2023
Final Technical Report

DISTRIBUTION A: Distribution approved for public release.

Air Force Research Laboratory
Air Force Office of Scientific Research
European Office of Aerospace Research and Development
Unit 4515 Box 14, APO AE 09421

REPORT DOCUMENTATION PAGE

PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ORGANIZATION.

1. REPORT DATE	**2. REPORT TYPE**	**3. DATES COVERED**	
20230228	Final	**START DATE** 20180924	**END DATE** 20220923

4. TITLE AND SUBTITLE
Fundamentals of Deformation Mechanisms in Polycrystalline Superalloys

5a. CONTRACT NUMBER	**5b. GRANT NUMBER**	**5c. PROGRAM ELEMENT NUMBER**
	FA9550-18-1-7000	61102F
5d. PROJECT NUMBER	**5e. TASK NUMBER**	**5f. WORK UNIT NUMBER**

6. AUTHOR(S)
Roger Reed

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
THE UNIVERSITY OF OXFORD
UNIVERSITY OFFICES
OXFORD
GB

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	**10. SPONSOR/MONITOR'S ACRONYM(S)**	**11. SPONSOR/MONITOR'S REPORT NUMBER(S)**
EOARD UNIT 4515 APO AE 09421-4515	AFRL/AFOSR IOE	AFRL-AFOSR-UK-TR-2023-0042

12. DISTRIBUTION/AVAILABILITY STATEMENT
A Distribution Unlimited: PB Public Release

13. SUPPLEMENTARY NOTES

14. ABSTRACT
This report summarizes the progress made on the project FA9550-18-1-7000 from 2018 to 2022. The project has built a US-UK international collaboration on the deformation (yielding, creep, fatigue) mechanisms in the high-strength nickel-based superalloys used for turbine applications.
The science of the time-dependent deformation mechanisms which are precursors to fatigue failure has been studied on new grades of superalloys carefully designed and selected for this project. The scientific aim was to better understand the mechanisms of deformation with atomic-scale chemical resolution.
Several scientific advances have been achieved through this project, including a new understanding of the high-temperature failure of the APB and Complex Fault strengthening mechanism in Ni-based superalloys. Also the d development of multi-scale modelling approach for the prediction of mid-temperature mechanical properties in Ni-based superalloys. Several papers were published and are listed in the report.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**	SAR	5
U	U	U		

19a. NAME OF RESPONSIBLE PERSON	**19b. PHONE NUMBER** *(Include area code)*
DAVID SWANSON	785-6565

Standard Form 298 (Rev.5/2020)
Prescribed by ANSI Std. Z39.18

FA9550-18-1-7000
Fundamentals of Deformation Mechanisms in Polycrystalline Superalloys

Principal Investigator: Prof. Roger C. Reed (University of Oxford)
Researchers: Dr. D. Barba, Dr. Y. Gong, Dr. Y. Tang, Dr. S. Utada

Final Report

Table of Contents

1. Executive Summary

This report sumarise the progress made on the project FA9550-18-1-7000 from 2018 to 2022. The project has built a US-UK international collaboration on the deformation (yielding, creep, fatigue) mechanisms in the high-strength nickel-based superalloys used for turbine applications, e.g. for jet engines, and especially the grades used for turbine discs [Reed 2006, Smith 2016a, Barba 2017a]. To ensure the best performance and fuel efficiency targets, temperatures are rising due to technical, commercial and legislative pressures [Reed 2006, The jet engine 2015]; the rims of the turbine discs are now experiencing temperatures of beyond 800°C in service [The jet engine 2015], a stress of many hundred MPa and become critical regions because the turbine blades are located in them. At these conditions, new deformation mechanics are appearing which combine the dislocation shearing common to low temperature with the segregation processes characteristic of high-temperature plasticity. When the project started in 2018, these mechanisms were far from being understood limiting the technological advance of turbine systems.

Two leading groups led by (i) Professor Roger Reed at Oxford – whose expertise relates to alloy design, numerical modelling and manufacturing [Crudden 2014, Turner 2011, Alabort 2015] – and (ii) Professor Mike Mills at The Ohio State University (OSU) – an expert in high resolution microscopy and deformation mechanisms in these materials [Phillips 2013, Dimiduk 2013, McAllister 2016] – have collaborated in this project to solve this problem. The science of the time-dependent deformation mechanisms which are precursors to fatigue failure [Kanesund 2011, Lv (2014), Barba 2017b, Smith et al. 2016b] has being studied on new grades of superalloys carefully designed and selected for this project jointly on both sides of the North Atlantic. The scientific aim was to better understand the mechanisms of deformation with atomic-scale chemical resolution – using pioneering approaches of OSU - and to build modelling capability for predictive purposes, for which Reed's group at Oxford is world-leading. The technological aim was to aid in the isolation of better grades of alloy with superior properties; thus, impact is anticipated via the modelling-driven design of improved alloys for these applications, so that improved engine technologies can be delivered.

2. Scientific Highlights

The most relevant scientific advances produced by this project can be summarised in the following:

- **New understanding of the high-temperature failure of the APB and Complex Fault strengthening mechanism in Ni-based superalloys.**
  In this project, the mechanism transition from room temperature to 900°C of the single crystal superalloy MD2 (similar to CMSX-4) has been studied systematically combining mechanical testing, cutting edge atomic scale characterisation and computational modelling. Thanks to a carefully designed experimental campaign, the mechanism transition behind the strength failure of this alloy after 750°C has been monitored. The transition of mechanisms as temperature increases has been rationalised by the use of atomic scale simulations (density functional theory).

- **Development of multi-scale modelling approach for the prediction of mid-temperature mechanical properties in Ni-based superalloys.**
  During this project, a multiscale modelling approach to link the alloy composition at the atomic scale with the mid-temperature creep performance has been developed. This link is stablished through the effect of alloy composition on the energy associated with the variety of fault forming in superalloys (obtained by means of DFT simulations)

and on the diffusional processes studied experimentally associated with the segregation to these faults (modelled by crystal plasticity theory). The multi-scale model has been used to analyse the transition of mechanical properties in a Ni-based superalloy from room temperature to 900°C

- **Mechanistic understanding of the effect of alloy composition on the mid-temperature creep performance in Ni-based superalloys**
  In this project, correlative high resolution transmission electron microscopy and energy-dispersive X-ray spectroscopy has been used to study the deformation faults in three different polycristalline Ni-based superalloys with carefully designed ratios of disordering-to-ordering-promoting elements (Co-Cr against Nb-Ta-Ti). These alloys have been carefully processed so the only microstructural and material difference was the alloy composition (e.g., same grain size, precipitate distribution). The results shows that the additions of ordering-promoting elements reduce the diffusional activity around the faults required for the faults to lengthen and thicken thus reducing the creep rates. These insights provide a path to follow in the design of improved grades of creep-resistant polycrystalline alloys beyond 700°C.

3. Scientific Publications

The results raised from this project has been published in scientific articles in top journals of the field. These articles have been highly cited by the community which is a proof of the strong interest of the community by the research produced within this project. The following articles in open-source mode has been published:

- Barba, D., Egan, A., Utada, S., Gong, Y., Tang, Y. T., Mazanova, V., ... & Reed, R. C. (2023). Deformation Mechanisms Rationalisation to Design for Creep Resistance in Polycrystalline Ni-Based Superalloys. *Metallurgical and Materials Transactions A*, 1-16.
  https://link.springer.com/article/10.1007/s11661-022-06922-9

- Barba, D., Egan, A. J., Gong, Y., Mills, M. J., & Reed, R. C. (2020, August). Rationalisation of the micromechanisms behind the high-temperature strength limit in single-crystal nickel-based superalloys. In *Superalloys 2020: Proceedings of the 14th International Symposium on Superalloys* (pp. 260-272). Cham: Springer International Publishing.
  https://link.springer.com/chapter/10.1007/978-3-030-51834-9_25

- Barba, D., Smith, T. M., Miao, J., Mills, M. J., & Reed, R. C. (2018). Segregation-assisted plasticity in Ni-based superalloys. Metallurgical and Materials Transactions A, 49, 4173-4185.
  https://link.springer.com/article/10.1007/s11661-018-4567-6#Ack1

Commented [d1]: If there is any further paper

4. Conference Presentations

Commented [d2]: Please add any further ones you might have go related to what the project is about.

The scientific outcomes of this project have been shared to the scientific community of the field in multiple international events:

- **TMS 2023**
  Creep Assisted Phase Transformation Deformation Mechanisms in Polycrystalline Ni-based Superalloys and Their Impact on the Creep Performance
  D. Barba; Ashton J. Egan; Satoshi Utada; Yilun Gong; Yuanbo Tang; Veronika Mazanova; Michael J. Mills; Roger C. Reed

TMS2023, March 2023, San Diego, USA

- **EUROSUPERALLOYS 2022**
  Deformation mechanisms rationalisation to design for creep resistance in polycrystalline Ni-based superalloys.
  D. Barba, A. Egan, S. Utada, Y. Gong, Y. T. Tang, V. Mazanova, M. J. Mills & R. C. Reed.
  Eurosuperalloys September 2022, Germany

- **TMS 2020**
  On the Temperature Limits of Ni-based Superalloys
  D. Barba, Ashton Egan; Michael Mills; Roger Reed
  TMS2020, February 2020, San Diego USA.

- **SUPERALLOYS 2021**
  Rationalisation of the micromechanisms behind the high-temperature strength limit in single-crystal nickel-based superalloy.
  D. Barba, A. Egan, S. Utada, Y. Gong, Y. T. Tang, V. Mazanova, M. J. Mills & R. C. Reed.
  Superalloys 2020, September 2021, USA (Online Event)

- **EUROSUPERALLOYS 2018**
  Deformation mechanisms rationalisation to design for creep resistance in polycrystalline Ni-based superalloys.
  Barba, D., Smith, T. M., Miao, J., Mills, M. J., & Reed, R. C
  Eurosuperalloys September 2018, Oxford

5. Acknowledgements

The researchers that participated in this project are thankful for the opportunity provided by the USAF Research Office under the grant FA9550- 18-1-7000. The sponsorship of the USAF Research Office has strengthened the collaboration between both parts of the Atlantic (Oxford and Ohio State University) through multiple jointly publications and disseminations to the superalloys field which have attracted an strong attraction.