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Multiresolution mechanical characterization of Ti alloys using spherical indentation stress-strain protocols and Bayesian inference of single crystal elastic-plastic properties

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<b>14. ABSTRACT</b> This project has successfully developed and demonstrated novel protocols for estimating the most important crystal level elastic-plastic properties for a large range of a-Ti alloys at different material length/structure scales. The data gathered from these protocols provided valuable quantitative insights into the dependence of salient microstructure features on the multiresolution properties exhibited by the different alloys. These tasks were accomplished using a combination of (i) multiresolution measurements of local mechanical responses using spherical indentation stress-strain protocols (with indented zone size varied systematically in the range of 50 nm to 500 microns), (ii) corresponding multiresolution characterization of the material structure at the relevant length scales using electron microscopy and back-scattered diffraction, (iii) multiresolution simulations of the indentation experiments using crystal plasticity finite element models, and (iv) estimations of the desired fundamental material properties at different length scales by matching the measurements and corresponding simulations using a suitable statistical learning approach with uncertainty quantification. The unique datasets and tools produced in this work have opened completely new avenues of research into multiscale studies of heterogeneous material systems, spanning the material and component length scales.			
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## **Multiresolution mechanical characterization of Ti alloys using spherical indentation stress-strain protocols and Bayesian inference of single crystal elastic-plastic properties**

### **Accomplishments**

Research Objectives: The central objective of this project is to develop and demonstrate novel protocols for establishing, with quantified levels of uncertainty, some of the most important crystal level elastic-plastic model forms and properties for a range of  $\alpha$ - $\beta$  Ti alloys at different material length/structure scales. Additionally, we will establish the functional dependence of these properties on the relevant quantitative measures of microstructure at each scale (e.g., chemical composition, lath thickness and spacing, colony size, and prior  $\beta$  grain size). The crystal level elastic-plastic model forms and parameters targeted in this study include (a) the elastic response of various microscale constituents found in Ti alloys, and (b) the effective resistances of the active slip modes in these complex material structures. These tasks are being accomplished using a combination of (i) multiresolution measurements of local mechanical responses using novel spherical indentation stress-strain protocols (with indented zone size varied systematically in the range of 50 nm to 500  $\mu$ m), (ii) corresponding multiresolution characterization of the material structure at the relevant length scales using electron microscopy and back-scattered diffraction, (iii) multiresolution simulations of the indentation experiments using crystal plasticity finite element models, and (iv) extraction of the appropriate model forms for strength, including the role of interfaces, and desired fundamental properties listed above by matching the measurements and corresponding simulations using a suitable statistical learning approach with uncertainty quantification.

Accomplishments During the Reporting Period: Since the accomplishments in prior years were reported in prior year reports, this report focusses only on the work performed in the last year of the project. This last year was a no-cost extension year for the project. As such, our goal was to finish the projects and write up our results into journal articles. The following significant activities and results/key outcomes resulted from this year's work:

- *Extension and application of the spherical indentation stress-strain protocols on lamellar and basket-weave grains in  $\alpha$ -Ti alloys.* We have successfully extended the novel spherical indentation protocols we developed, demonstrated, and published on the primary  $\alpha$  grains in prior years to both the lamellar and basket-weave grains. The key insights from these studies include: (i) The elastic and plastic response of colony alpha-beta is substantially different than that of primary alpha. A dip in the indentation yield properties at 45 degrees declination angle is observed, along with a reduction of elastic anisotropy. A journal publication describing these measurements and analyses is being currently prepared for a journal publication. (ii) The basket-weave morphology, comprising of retained beta and secondary alpha phases in the form of platelets that form a characteristic triangular pattern, produces an effective (i.e., homogenized) grain-scale response that can be adequately captured using isotropic plasticity models. However, the details of the basket-weave lath morphology (e.g., lath thickness, lath spacing) had a significant effect on their grain-scale

effective response. Generally, samples with coarser lath microstructures were found to exhibit lower strengths. One paper describing these results has already been published (details provided in the publication list added to this report), and another paper is currently being prepared for a journal publication.

- *Development of a new framework for the extraction of model parameters and the computation of model form probabilities.* We have extended the two-step Bayesian framework developed, utilized, and published in the prior year effort in two important ways: (i) Application of the framework to significantly more complex material models at the grain-scale with a significantly larger number of model parameters that need to be calibrated to limited uncertain experimental observations. (ii) Objective assessment of probabilities for alternate candidate models for fitting the available limited and uncertain experimental observations. Specifically, we focused on the estimation of the intrinsic colony-scale effective plastic properties (i.e., CRSS values) of lamellar and basket-weave ( $\alpha+\beta$ ) grains. One paper describing these results has already been published (details provided in the publication list added to this report), and another paper is currently being prepared for a journal publication.
- *Further Development of Small Punch Test (SPT) Protocols.* Building on prior year's published effort, we dramatically improved the analyses protocols for converting the measured load-displacement curves in SPT to the much more readily interpretable uniaxial (i.e., simple compression) stress-strain curves. This was accomplished by extending the 2-step Bayesian framework developed in the prior year effort. Additionally, the Swift strain hardening law used in the prior year effort was replaced with the Voce hardening law to allow for a better representation of the measured stress-strain responses in most metal alloys. The results and conclusions from this effort are being currently prepared for a journal publication.

Dissemination of Results: As already described earlier, we are in the process of writing up journal papers describing our results. Additionally, we have also shared our datasets and codes in open-source repositories. These have included:

- Use of spherical nanoindentation protocols to study the anisotropic mechanical response of alpha-beta single colonies in Ti-6Al-4V alloy, NIST Materials Data Repository, <https://hdl.handle.net/11256/995>, 2021.
- N. Millan, S. Mohan, A. Pilchak, and S. R. Kalidindi, "Spherical nanoindentation stress-strain curves of primary- $\alpha$  grains in Ti5-2.5, Ti811, Ti64, Ti6242 and Ti6246 alloys", NIST Materials Data Repository, <https://hdl.handle.net/11256/989>, 2020.
- PyMKS <http://pymks.org/>
- Spherical nanoindentation stress-strain analysis at <https://github.com/jsweaver/Spin>
- Materials Data Hub <https://materialhub.org/>

Additionally, the PI has helped launch a new venture-funded start-up funded by Micron Ventures. The start-up called Multiscale Technologies, Inc., has just released its pilot version of a new commercial materials data science and AI platform that will serve its customers by dramatically accelerating their materials innovation efforts. Some of the students who worked on the AFOSR project are now employed with the start-up, offering new avenues for commercial translation of their research.

## **Impacts**

Development of the principal discipline(s) of the project: This study is critical to the advancement of new materials design rules and development methods for  $\alpha$ - $\beta$  Ti alloys in the efforts to meet the demands of critical aerospace applications.  $\alpha$ - $\beta$  Ti alloys exhibit high strength to weight ratios with excellent corrosion resistance and fatigue properties needed for many aerospace applications. This project has pioneered the development of highly efficient workflows for optimally producing the computational and experimental datasets needed to support the rational, dramatically accelerated, design and development of these advanced alloys for the US Air Force.

Development of human resources: The project has contributed to the professional development of one female post-doctoral student and four graduate students (one female and three male students; two of them also belong to underrepresented groups). This group of young researchers were trained in cross-disciplinary research involving advanced concepts and tools in mechanics of materials, materials science, data science, and computer science. Furthermore, the students were also exposed to the state-of-the-art tools in both mechanics of materials experiments and multiscale physics-based simulations. One of the students is now employed by Blue Origin in Kent, WA.

Impact on teaching and educational experiences: The PI has co-designed and co-taught, with Prof. Yan Wang, a new graduate course titled “ME8813: Machine Learning Fundamentals for Mechanical Engineering”. The advances made in this research project contributed significantly to the content and design of this new course. This course was offered for the very first time in Spring 2022. We had 90 students registered for the class. This course will become a foundational course in a new graduate certificate program to be developed at GT (Georgia Tech) centered around AI/ML applications for mechanical engineers. Given how AI/ML have already impacted various fields of sciences and technology, I am confident that this new course and the new graduate programs to be developed at GT will have a broad positive and beneficial impact on future students, industrial partners, and the broader professional scientific community in the long term.

## **Changes**

Nothing to report.

## **Technical Updates**

Nothing more to report.