RX21-23

1. **Research Title:** Dynamic prediction of grain size distribution evolution during hot deformation

2. **Individual Sponsor:**

Dr. Eric J. Payton, AFRL/RXCM
Building 655, Rm 084
2230 Tenth St
WPAFB, OH 45433
eric.payton@us.af.mil

3. **Academic Area/Field and Education Level**

Materials Science & Engineering / Modeling & Simulation in Materials Science
(MS, PhD level)

4. **Objectives:** Predict the new grain nucleation rate during dynamic recrystallization in two phase alloys when grain boundary sliding is an active strain accommodation mechanism.

5. **Description:** Recent research has revealed that the barrier to nucleation for new grains may be suppressed during recrystallization in the presence of a coherent or semi-coherent secondary phase from which the recrystallization nuclei can template epitaxially [1,2]. This mechanism appears to be active during thermomechanical processing of key aerospace alloys in both the Ni- and Ti- base systems, and may play an important role in the development of the size and spatial distributions of the microstructural features. It appears possible that some of the challenges in accurately predicting grain size after processing may stem from not taking this phenomena into account. Now that simulation methodologies combining phase field with Potts Monte Carlo modeling [3] and full-field crystal plasticity finite element modeling [4] are available, realistic direct simulations of microstructure evolution at elevated temperatures are becoming feasible. In the case of Ni-base superalloys and the workhorse Ti alloy, Ti-6Al-4V, interface sliding is an important strain accommodation mechanism at relevant processing temperatures. Interface sliding is accommodated by motion of crystalline interface defects known as disconnections [5] and accompanied by shear-coupled boundary motion. The physical mechanisms of grain boundary sliding must therefore be incorporated into simulation methodologies to advance our predictions of microstructure evolution during processing of engineering alloys for aerospace applications. This project aims to advance the state of the art for direct simulation of microstructure evolution in processing regimes where interface sliding and dynamic recrystallization are active, then apply this simulation methodology toward predicting the spatial distribution of recrystallization nuclei and their nucleation rate during elevated temperature deformation. It is anticipated that predictions of the conditions under which the spatial density of nuclei are low and local crystalline defect storage is high will help pinpoint processing regimes where formation of coarse grains (which are detrimental to fatigue life) are likely to occur.

6. **Research Classification/Restrictions:** This research topic is unclassified basic research eligible for publication in the open literature.

7. **Eligible Research Institutions:** Wright State University, Ohio State University, University of Dayton, Miami University, Ohio University, University of Cincinnati, Air Force Institute of Technology

References

[1] V. Miller, E. Payton, A. Pilchak, "Reduction in the thermodynamic nucleation barrier via the heteroepitaxial recrystallization mechanism." Scripta Materialia 136 (2017) 128–131.

[2] S. Balachandran, S. Kumar, D. Banerjee, "On recrystallization of the alpha and beta phases in titanium alloys." Acta Materialia 131 (2017) 423–434.

[3] E. R. Homer, V. Tikare, E. A. Holm. "Hybrid Potts-phase field model for coupled microstructural-composition evolution." Computational Materials Science 69 (2013) 414—423.

[4] D. A. Ruiz Sarrazola, L. Maire, C. Moussa, N. Bozzolo, D. Pino Munoz, M. Bernacki. "Full field modeling of dynamic recrystallization in a CPFEM context – Application to 304L steel." Computational Materials Science 184 (2020) *in press.*

[5] C. Wei, S. L. Thomas, J. Han, D. J. Srolovitz, Y. Xiang. "A continuum multi-disconnection-mode model for grain boundary migration." J. Mech. Phys. Solids 133 (2019) 103731.