RX17-10

First Principles Calculations of Creep Mechanisms

1. **Research Title:** First Principles Calculations of Creep Mechanisms
2. **Individual Sponsor:**

Dr. Christopher Woodward AFRL/RXCM
Building 655, rm 089
2230 Tenth St.
WPAFB, OH 45433-7817
christopher.woodward@us.af.mil

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

   Materials Science, Physics, Computer Science (MS, PhD level)

4. **Objectives:** Predict the rate limiting kinetics behavior of high temperature creep mechanisms in Ni-based superalloys.
5. **Description:** Several high temperature creep mechanisms in Ni-based superalloys have been associated with diffusion in and around the super-dislocations in Ni_3Al precipitates. In this work a unique first principles boundary condition method will be used to isolate the super-dislocation cores and calculate the diffusion of various chemical species in the leading partial dislocations. Predicted diffusion rates can then be used to suggest changes in alloy chemistry to mediate this creep mechanism. Activation pathways for micro-twinning nucleation and growth may also be explored using atomistic methods.
6. **Research Classification/Restrictions:** This research topic is basic research and will be published in the open literature.
7. **Eligible Research Institutions:** Indicate to what organizations this topic should be provided

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