

DOE-ID NEPA CX DETERMINATION

Idaho National Laboratory

SECTION A. Project Title: Understanding non-equilibrium, nanoscale defects in bulk metals

SECTION B. Project Description and Purpose:

Radiation effects in materials are a concern for any structure exposed to ionizing radiation. Nuclear power applications, accelerators, space nuclear applications, and isotope production facilities all share a common concern of materials property changes during exposure to radiation. Neutron, ion, and even electron radiation can transfer energy to atoms in a crystalline lattice and, if the transferred energy exceeds the displacement energy of the atom, an atomic displacement is produced leading to vacancies and interstitials. The quantity of vacancies and interstitials produced depends on the type of radiation (mass of the particle), incoming energy, and the host material. Following the initial displacement, only a fraction of the generated vacancies and interstitials remain and build up to a non-equilibrium steady state concentration of point defects. After the irradiation, when defect generation ceases, both the vacancy and interstitial content reduces further, striving for thermodynamic equilibrium. However, it is this initial non-equilibrium defect concentration that is responsible for the formation of larger defects such as voids or dislocation loops, which in turn may significantly alter the material's properties. Therefore, understanding and quantifying the non-equilibrium defects in a material is key to predicting long-term property change. The project is focused on developing the science basis for synthesizing and characterization chemically-complex actinide thin films and heterostructure. This work proposes to use pulsed ion beam irradiation to generate transient elevated populations of nanoscale defects in pure, single crystal nickel while using in situ laser metrology to continuously capture the resulting change in elastic moduli, which are sensitive to both vacancies and interstitial.

This project plans to generate baseline experimental data on transient nanoscale defect populations in bulk nickel (Ni) as model FCC metal through in situ pulsed ion beam exposure. The project involves the use of the unique capability to monitor material properties (elasticity and thermal transport) in situ during ion beam exposure at Center for Integrated Nanotechnologies (CINT). Recent work focusing on the effects of transient defect populations in Ni-based concentrated solid solution alloys (CSAs) showed rich behavior as a function of ion flux and defect generation rate at a fixed temperature across alloy compositions. To benchmark both classical defect generation and recombination theory, as well as more sophisticated kinetic Monte Carlo (KMC) and cluster dynamics (CD) methods, the coupled effects of nanoscale defects of different characters (interstitial- or vacancy-type) will be explored in bulk pure Ni as a model system at a variety of temperatures, defect generation rates, and annealing times. Such fundamental data will not only serve as a unique benchmark for increasingly-used computational tools, it will also provide a direct baseline for new in situ capabilities coupling positron annihilation spectroscopy (PAS) and defect generation through ion beam exposure. The research will take place in INL Research Center (IRC) Laboratories C10, B17, and B3.

This single crystal, >99.99% purity Ni substrates will be sourced commercially. These substrates will be subjected to bench-top transient grading spectroscopy (TGS) examination using the experimental apparatus in the laboratory to determine relative crystal orientation, baseline material elastic properties, and baseline thermal transport properties. A series of exposure temperatures, dose rates, and annealing times for in situ pulsed irradiation experiments will be determined using rate theory to ensure that a large selection of transient defect levels are explored. Feasible temperatures range from 300-600°C based on the user facility, which will ultimately set the limits for the dose rates and annealing times chosen. All handling remains the same as any commercial metal following these exposures. These samples remain in our historical sample catalogue following the work described in this project. There will be no radioactive waste or hazardous waste produced. Only a generation of approximately 1 square foot of industrial waste such as cardboard, plastic, etc., will be produced. Once baseline measurements are made in the Laboratory and the experimental parameter is selection complete, in situ irradiation experiments will take place at CINT targeting:

- A total of 5 irradiation temperatures in the range 300-600°C (and higher temperatures if facility upgrades take place).
- A total of 8 dose rates (defect generation rates) at each selected temperature, logarithmically sampled. The upper limit in dose rate will be set to $5 \cdot 10^{-3}$ dpa/s to limit excess heating from the ion beam.
- Sufficient annealing time between each irradiation pulse to ensure baseline properties have been recovered. Annealing times will vary at each temperature to ensure a defect-free reference is available for each impulse. Through each of these steps, collaborators at UC Berkeley will estimate the expected point vacancy and interstitial concentrations at the temperatures and dose rates selected. The scope of this project will be limited to the experimental collection and simple rate modeling of the defects observed in these transient conditions. If successful, follow-on work will be undertaken to calculate the same quantities (time-dependent defect populations) using more advanced cluster dynamics formulations. While the experimental infrastructure to conduct this study is located at a large-scale facility outside of the Laboratory, it is the unique expertise in laser metrology and defect dynamics of scientists here Idaho National Laboratory (INL) that will allow the construction of these test matrices, the practical implementation of the experimental scope, and the eventual interpretation of the dynamic responses.

All handling remains the same as any commercial metal following these exposures. The samples will remain in the historical sample catalogue following the work described in this project.

SECTION C. Environmental Aspects or Potential Sources of Impact:

Air Emissions

N/A

Discharging to Surface-, Storm-, or Ground Water

N/A

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Disturbing Cultural or Biological Resources

N/A

Generating and Managing Waste

Generation of waste includes packaging materials such as cardboard, plastic, etc., from Ni substrates being sourced commercially. The amount of waste that will be generated will be less than 1 foot squared of industrial waste.

Releasing Contaminants

Laboratory personnel would maintain chemical inventories to verify compliance with applicable codes, standards, and regulations.

Using, Reusing, and Conserving Natural Resources

All materials will be reused and recycled where economically practicable. All applicable waste will be diverted from disposal in the landfill where conditions allow.

SECTION D. Determine Recommended Level of Environmental Review, Identify Reference(s), and State Justification: Identify the applicable categorical exclusion from 10 Code of Federal Regulation (CFR) 1021, Appendix B, give the appropriate justification, and the approval date.
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For Categorical Exclusions (CXs), the proposed action must not: (1) threaten a violation of applicable statutory, regulatory, or permit requirements for environmental, safety, and health, or similar requirements of Department of Energy (DOE) or Executive Orders; (2) require siting and construction or major expansion of waste storage, disposal, recovery, or treatment or facilities; (3) disturb hazardous substances, pollutants, contaminants, or Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)-excluded petroleum and natural gas products that pre-exist in the environment such that there would be uncontrolled or unpermitted releases; (4) have the potential to cause significant impacts on environmentally sensitive resources (see 10 CFR 1021). In addition, no extraordinary circumstances related to the proposal exist that would affect the significance of the action. In addition, the action is not "connected" to other action actions (40 CFR 1508.25(a)(1) and is not related to other actions with individually insignificant but cumulatively significant impacts (40 CFR 1608.27(b)(7)).

References: 10 CFR 1021, Appendix B to subpart D, items B3.6, "Small-scale research and development, laboratory operations, and pilot projects"

Justification: Irradiation B3.6 Small-scale research and development, laboratory operations, and pilot projects. Siting, construction, modification, operation, and decommissioning of facilities for small-scale research and development projects; conventional laboratory operations (such as preparation of chemical standards and sample analysis); and small-scale pilot projects (generally less than 2 years) frequently conducted to verify a concept before demonstration actions, provided that construction or modification would be within or contiguous to a previously disturbed or developed area (where active utilities and currently used roads are readily accessible). Not included in this category are demonstration actions, meaning actions that are undertaken at a scale to show whether a technology would be viable on a larger scale and suitable for commercial deployment

Is the project funded by the American Recovery and Reinvestment Act of 2009 (Recovery Act) Yes No

Approved by Jason L. Anderson, DOE-ID NEPA Compliance Officer on: 10/25/2021