Proposal ID Number: 19841
Title of Proposal: Defects and Defect Processes in Ceramics
PI: William Weber
Institution: Pacific Northwest National Laboratory

Description of Work:
The proposed work is to develop fundamental understanding of defects, defect processes and interfaces in ceramics at the atomic level. In addition, the work will focus on the role of interfaces on dynamic phase transitions and on electronic, ionic, defect and gas transport properties in materials relevant to environmental, energy and national security missions. The work will focus on surface/interface properties; include radiation effects, defect-interface interactions and transport, the role of hydrogen and surface structure on electronic and ionic transport. This work is relevant to nuclear waste immobilization, the hydrogen economy, fuel cell technology, materials for a closed nuclear fuel cycle, materials for advanced nuclear power technology, and advanced radiation detector technology. The proposal will employ multiple experimental facilities and techniques in EMSL.

The defect processes of primary interest are defect production and formation, defect migration, defect interactions, and defect mechanisms related to the kinetics of irradiation effects, ion implantation, ionic transport, and phase transformations in ceramics. The research approach and management philosophy are based on a team of highly-motivated experimental at PNNL and external collaborators who perform highly-integrated studies with computational scientists on defects and defect processes in related materials.

Results:
Major breakthroughs have been obtained in understanding defects, defect processes, the evolution of nanostructures, and the role of ionization in dynamic defect recovery and recrystallization in silicon carbide, gallium nitride, aluminum nitride, rare-earth apatites, and gadolinium titanate-zirconate. The behavior of atomic defects, nanostructure evolution, and the impact on performance can be predicted with more confidence in these materials. By tailoring defects and nanostructures, durable devices and components can be produced that enable technological advances in energy efficiency, national security, energy production, and medical applications.

Awards/Recognition:
William J. Weber – 2006 *Fellow of the American Association for the Advancement of Science*

Publications:
A list of publications is provided below. Most publications this past year were associated with prior project 3448 and 3448a.

1. Jiang W, Y Zhang, V Shutthanandan, S Thevuthasan, and WJ Weber. 2006. "Temperature response of 13C atoms in amorphized 6H-SiC." *Applied Physics Letters* 89(26):art. no.:261902, (3 pages). doi:10.1063/1.2422892

2. Bae I, Y Zhang, WJ Weber, M Higuchi, and L Giannuzzi. 2007. "Electron-beam induced recrystallization in amorphous apatite." *Applied Physics Letters* 90(2):021912, 1-3. doi:10.1063/1.2430779

3. Jiang W, I Bae, and WJ Weber. 2007. "Disordering and Dopant Behaviour in Au^+ Ion Irradiated AlN." *Journal of Physics. Condensed matter*. [In Press]

Request for Extension:
We are requesting a one-year extension to continue the long-term research objectives outlined in the original proposal. This will include continue ion-beam implantation, ion-beam analysis, electron microscopy, XPS, SIMS, and X-ray diffraction studies of silicon carbide, gallium nitride, aluminum nitride, zirconium carbide, zirconium oxide, cerium oxide, rare-earth silicates with the apatite structure, rare-earth titanate-zirconates with the defect fluorite or pyrochlore structure, and zinc oxide. We will also initiate in-situ characterization of defect production in single cascade events using the time-of-flight telescope and accompanying instrumentation. The resources requested for the next year are as follows:

- Ion-Accelerator Facility: 240 hours
- Electron Microscopy Facility: High-Resolution TEM: 240 hours
- Electron Microscopy Facility: Dual-Beam Focused Ion Beam (FIB/SEM): 240 hours
- Electron Microscopy Facility: Scanning Field Emission (LEO): 40 hours
- Digital Instrument (DI) Nanoscope IIIa multimode scannning probe microscope: 40 hours
- Electron Spectrometer: XPS High Resolution (Quantum): 40 hours
- Time-of-Flight Secondary Ion Mass Spectroscopy (ToF SIMS): 40 hours
- X-ray Diffraction Systems: 40 hours