# AC 2007-480: A SUCCESSFUL PROTOTYPE FOR UNIVERSITY/NATIONAL LABORATORY RESEARCH COOPERATION

**James Tulenko, University of Florida**

James S. Tulenko, a professor in the Department of Nuclear and Radiological Engineering at the University of Florida in Gainesville, Fl, is also the Director of the Laboratory for Development of Advanced Nuclear Fuels and Materials. He was Chairman of the Department of Nuclear and Radiological Engineering at the University of Florida for sixteen years. He is a Past President of the American Nuclear Society (ANS). Prior to his academic career, Professor Tulenko spent 23 years in the Nuclear Industry as Manager, Nuclear Fuel Engineering at Babcock and Wilcox; Manager of Physics at Nuclear Materials and Equipment Corp, and Manager, Nuclear Development at United Nuclear. He was an Adjunct Professor at Geo. Wash. University. Professor Tulenko was a teaching Fellow at Harvard University. Prof. Tulenko has numerous fields of interest in the nuclear area, most of which involve the nuclear fuel cycle. He was presented with the Silver Anniversary Award of the American Nuclear Society (ANS) for his contributions to the nuclear fuel cycle in the first 25 years of the ANS. He has also received the Mishma Award of the ANS for his nuclear material research. For his contributions to Nuclear Science and Technology he has received the Arthur Holly Compton Award of the ANS and the Glenn Murphy Award of the American Society for Engineering Education. He is a Fellow of the American Nuclear Society for his contributions to the nuclear fuel cycle. He is a past member of the National Nuclear Accrediting Board of the Institute of Nuclear Power Operations, Chairman of the Chemical Materials and Technology (CMT) Division Review Board at Argonne National Laboratory, and a member of the Advisory Review Board for the Decision Applications (DA) Division at Los Alamos National Laboratory. He is also an Associate at Los Alamos National Laboratory. He is a member of the Nuclear Advisory Board for the Nuclear Engineering Graduate Program at the University of South Carolina. He is a Commissioner of the Applied Science Accreditation Commission and a past Commissioner of the Engineering Accreditation Commission. He has authored sections on the nuclear fuel cycle in the Handbook of Mechanical Engineering and the Encyclopedia of Energy Engineering and Technology. He was an editor of the proceeding of "Intelligent Robotics and Remote Systems for the Nuclear Industry," and has published well over a hundred and fifty technical publications dealing with energy. He serves on the Editorial Advisory boards for the Journal of Nuclear Engineering and Science and the publication, Radwaste Solutions.

A Successful Prototype for University/National Laboratory Research Cooperation

The University of Florida has recently become a participant in a Department of Energy (DOE), Office of Energy's 'Computational Materials Science Network' (CMSN) Cooperative Research Team (CRT) program. From our experience with the program, we find that this type of program is an outstanding way to enhance University/ National Laboratory research cooperation. Successful CRTs are funded typically for three years at a level determined by DOE headquarters - currently $280K/year/team. Teams do not renew, although a team my reconstitute itself on a closely related problem. Individual participation in a CRT is determined by self-selection of the group of collaborators and is open to anyone who can contribute to the success of the team, including scientists from DOE labs, other U.S. government labs, universities, and industry. The mission of the Computational Materials Science Network is to advance frontiers in computational materials science by assembling diverse sets of researchers committed to working together to solve relevant materials problems that require cooperation across organizational and disciplinary boundaries. We feel that this program should serve as a prototype for the Office of Nuclear Energy Science and Technology to foster National Laboratory/University/Industry Collaboration.

The CMSN Program utilizes an integrated management approach. This model includes the use of large multidisciplinary laboratory, university and industry teams to focus on the development of standardized and optimized codes. A community wide management approach is utilized to dynamically set focus areas and assign appropriate financial resources to accomplishing goals. Finally, the network provides organizational structure that can articulate the goals of the team for the development and usage of technology resources.

The CMSN program that the University of Florida is participating in entitled "***Multi-scale Simulation of Thermo-mechanical Processes in Model Fission-Reactor Materials" subtitled 'Microstructure and Deformation Physic of Irradiated Materials'***

Dr. Dieter Wolf from the Idaho National Laboratory is the team organizer and director. The program has three subtasks with task leaders from both Universities and National Laboratories. The subtasks are: (1) Unit mechanisms in the thermo-mechanical response in nuclear materials, which is led by Los Alamos National Laboratory; (2) Coupled irradiation and thermo-mechanical behavior of nuclear materials with atomic-level resolution, which is led by the University of Florida and Pacific Northwest National

Laboratory and (3) Atomistically-informed mesoscale modeling of coupled irradiation and thermo-mechanical behavior of nuclear materials, which is lead by Idaho National Laboratory.. The CMSN team involves six DOE laboratories, five universities and NASA. The DOE laboratories are Idaho, Argonne, Los Alamos (LANL), Oak Ridge, Lawrence Livermore and Pacific Northwest National Laboratory (PNNL). The five schools are the Universities of Arizona, Florida, Florida State, Rensselaer, and M.I.T. The program has a Senior Scientific Advisory Committee. This is the committee on which I serve.

The team will split the $280K yearly funding, with 2/3 going to support graduate students and Post docs and 1/3 to hold two meetings each year and to provide funding support for collaboration of team members, their students and post-docs. The $200K for partial investigator (graduate students and post-docs) support is divided into six grants, composed of two $50K grants and for $25K grants. The University of Florida (UF) has been awarded two $25K grants to support graduate students during the first year of the project. One UF student is Taku Watanabe, who he is working on the thermal transport and radiation damage and the other student is Pankaj Nerikar, who is working on point defects in UO2.

Of the two meeting to be supported each year, one meeting is limited to the CRT team and will address the ongoing research and will review team funding requests and the other meeting is an open meeting designed to bring in outside experts in the field who can contribute to the success of the projects.

The scientific approach for the team will focus on UO2 fuel with Zircaloy (Zr) Cladding and will also consider inert matrix materials such as SiC and MgO. Under Subtask-1, the team (two laboratories and one university) will utilize electronic structure based methods and atomistics and will be lead by Blas Uberuaga of LANL. This team will study interactions between point defects and defect cluster formation and the interaction of point defects and defect clusters with both grain boundaries and dislocations. The team (six laboratories and three schools) for subtask-2 will utilize large scale molecular dynamics, kinetic Monte Carlo, accelerated molecular dynamics and hybrid methods and will be lead by Simon Philpot of UF and Ram Devnathan of PNNL. This team will study the effects of radiation damage on coupled grain growth and deformation at high temperature, the effect of radiation damage on thermal transport and mechanical properties, fission-gas bubble formation and evolution and its effect on thermo-mechanical properties and finally various aspects of cascade evolution. The team (fie laboratories and one school) for subtask-3 will utilize front-tracking combined with phase field and finite element to study a variety of subjects ranging form models of free energy

of phases and calculation of phase stability, simulation of phase transformation including nucleation, growth and species segregation, to interfacial chemistry effects of irradiation.

The success of the this project is measured in several ways. One obvious measure is the advancement of knowledge in the material science of nuclear materials with the development of new or extended atomistic material codes. Other important successes will be the development of a nucleus of researchers within the atomistic materials community who have come together across organizational boundaries. A measure will be if the team is successful in the development o collaborations to initiate joint funding proposal to carry out the work initiated here. The project will also provide a collaborative environment for the coming generation of atomistic material scientist in the nuclear area.

The project has already achieved a major success with the award of one of twelve cooperative research projects, under the Nuclear Energy Research Initiative (NERI). The UF proposal entitled "Fundamental Processes of Coupled Radiation Damage and Mechanical Behavior in Nuclear Fuel Materials for High Temperature Reactors" is led by Dr. Simon Philpot with the author as Co PI and includes Dr. Dieter Wolf of the Center for Advanced Modeling and Simulation (CAMS) at Idaho National Laboratory (Director of the CMSN program) and Dr. Blas Uberuaga of MST-SPR at LANL, who will be the formal collaborators on this project; and Dr. Kurt Sickafus of MST-SPR at LANL, who will provide a direct link to LANL's experimental programs on nuclear materials. All are members of the CMSN program to develop university national laboratory research ties. The main thrust of the proposed research is to combine state-of-the-art techniques for the simulation of radiation damage cascades at both short and long time scales with state-of-the-art techniques for the simulation of mechanical deformation. This integrated approach will provide a powerful tool to elucidate the fundamental interactions between radiation damage and mechanical properties in polycrystalline microstructures. It will be noted that this area was one of the areas called out for research in the CMSN program. The research contract is for three years and is funded at a level of $400,000 dollars, with all the funding going to UF. This award will further engage UF professors and their students in advanced nuclear fuel cycle research and development with the national laboratories. (R&D

In conclusion, this project has already served to foster extensive collaboration between the universities and DOE national laboratories, with several of our students spending a semester at the national laboratory working under the leadership of our national

laboratory participants. It is expected that extensive interactions between the universities and the national laboratories will be a direct result of this program, with several joint proposals already submitted for further funding by team members. A successful research collaboration in the first year of the program has resulted from one of the submittals generated by UF under this program.