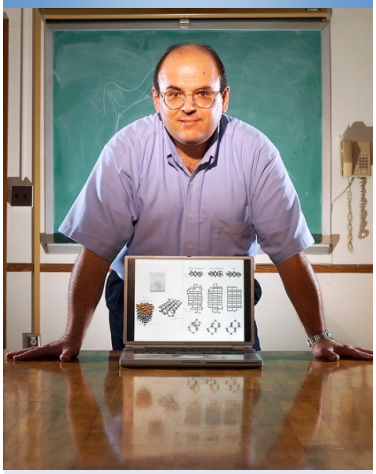
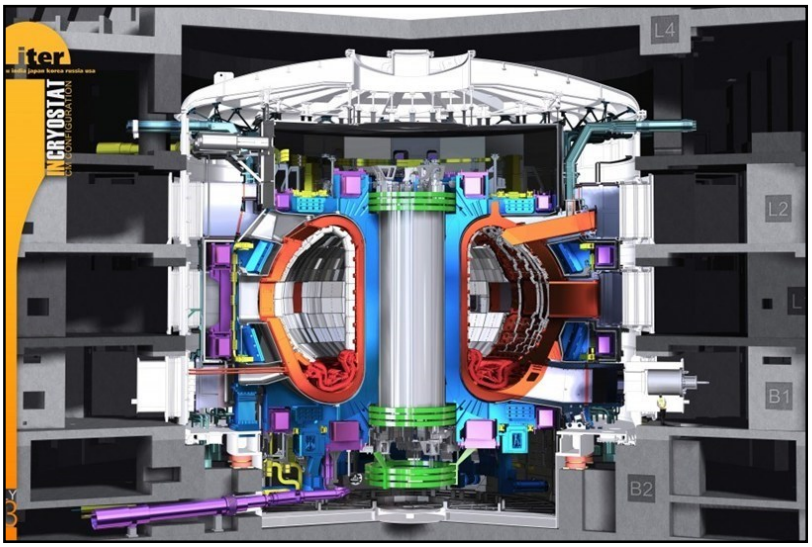
Research Continued...



DIMITRI MAROUDAS GIVES KEYNOTE LECTURE ON COMPUTATIONAL MATERIALS SCIENCE

Dimitri Maroudas was one of two keynote lecturers at the Second International Computational Science and Engineering Conference that took place in Doha, Qatar in October 2017. Prof. Maroudas' keynote lecture was entitled "Defect Engineering and Patterning of Crystal Surfaces, Epitaxial Thin Films, and Two-Dimensional Materials: A Computational Materials Science Approach". The presentation emphasized how computational materials science can help revolutionize materials processing and function, focusing on the exploitation of pattern forming instabilities on surfaces of crystals and epitaxial thin films to enable new nanofabrication technologies and on defect engineering of graphene derivatives and graphene-based carbon metamaterials.



Dimitri Maroudas is the UMass PI in multi-million, multi-institutional SciDAC Center on Plasma-Surface Interactions

Dimitri Maroudas is the UMass Amherst Principal Investigator (PI) on a new 5-year $19,600,000 SciDAC (Scientific Discovery through Advanced Computing) center on "Plasma-Surface Interactions: Predicting the Performance and Impact of Dynamic PFC Surfaces" awarded by the U.S. Department of Energy (DOE). This is a multi-institutional (six national laboratories, four research universities, and one company) research center funded by DOE's Offices of Fusion Energy Sciences and Advanced Scientific Computing Research and led by Prof. Brian D. Wirth of the University of Tennessee Knoxville and Oak Ridge National Laboratory. The new SciDAC centers were announced by DOE in the fall of 2017. This new center on plasma-surface interactions will build on the success of the team's previous 5-year $11,499,000 SciDAC center, where Prof. Maroudas also served as UMass PI, leading the team's surface physics research activities. SciDAC centers address grand-challenge ("big science, big computing") problems, and advance the state of the art in computational science utilizing leadership-scale computing facilities.

The objective of this center is to develop, and integrate, high-performance simulation tools capable of predicting plasma facing component (PFC) operating lifetime and the impact of the evolving surface morphology and composition of tungsten-based PFCs on plasma contamination, including the dynamic recycling of fuel species and tritium retention, in future magnetic fusion devices. This project will enable discovery of phenomena controlling critical PFC performance issues, and quantitatively predict their impact on both steady-state and transient plasma conditions. The outcome of this project will be a suite of coupled plasma and materials modeling tools, and a leadership class PFC simulator to predict PFC evolution and feedback to the boundary plasma. Success in the proposed research tasks will enable the prediction of both plasma fueling and the sources of impurity contamination that impact core plasma performance, and will lay the foundation for understanding, designing and developing the materials required to meet the performance objectives of future fusion reactors. The image above is a schematic of the International Thermonuclear Experimental Reactor (ITER). Nuclear fusion is a widely recognized grand challenge for science and engineering in the 21st century.

Research in Prof. Maroudas' group at UMass, within this center, will focus on developing models and simulation tools to predict PFC surface morphological evolution and near-surface structural evolution and to evaluate how such dynamical response affects thermomechanical PFC materials properties, including thermal conductivity, elastic properties, and mechanical strength. The research will involve a comprehensive suite of first-principles and classical computational statistical mechanical simulators, as well as rigorous hierarchical (atomistically informed), multiscale models of surface and atomic transport and plasma-exposed materials kinetics.