

**MMSNF-2003**

**Second Call**

# **Materials Modeling and Simulations for Nuclear Fuels**

**June 9-10, 2003**

**Santa Fe, New Mexico, U. S. A.**



Organized by Los Alamos National Laboratory  
Los Alamos, NM 87545, U. S. A.

**SCOPE:** The Workshop aims at stimulating research and discussions on modeling properties of ceramic and metallic fuels and related materials of interest for the Nuclear Fuels applications. Multi-scale models and simulations, involving various methods, such as CALPHAD, SOLGASMIX, Finite Element Method, Molecular Dynamics, Monte Carlo and First Principles calculations are welcomed. Presentation of experimental results in support of modeling and simulation is encouraged.

**Preliminary agenda (abstracts still accepted!):**

- Ed Arthur, NTA Office, *The Six Laboratory Director Nuclear Initiative -- How Advanced Fuels Development Supports Its Objective.*
- K. Chidester, LANL, *Coupling Experiments and Simulations for Designing Materials for Nuclear Fuels.*
- J. Tulenko, Univ. of Florida, *FRAPCON: A Computer Code for the Calculation of Steady-State, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup.*
- M. I. Baskes, LANL *The Role of Atomistic Modeling in Designing Materials.*
- R. Grimes et. al, Imperial College, UK, "*Fission product accommodation and containment*".
- P. Mason et al., AEA Technology, US/UK, *Solidus and liquidus determinations for a  $UO_{2+x}$ - $ZrO_2$  mixture.*
- Mikael Jolkkonen, KTH, Sweden, *Decarburisation reactions modelled using Thermo-Calc and the ALCHYMY database for uranium-free fuels.*
- M. Stan, LANL, *Phase Stability in Materials for Nuclear Fuels Applications.*
- David W. Price, AWE, UK, *Molecular Modelling Studies of Transport Phenomena in  $UO_2$ .*
- Wai-Yim Ching, Univ. of Missouri-Kansas City, *Spectroscopic Signatures of Defected Ceramics.*
- S. M. Valone et al. LANL, *Charge Fluctuation Models for Nuclear Fuels Properties.*
- J. Wills, LANL, *Prediction of materials properties for nuclear fuels from First Principles Calculations.*
- I. Han et al., Arizona State Univ. *Micro-hardness, Fracture Toughness, Fatigue and Texture Development in Sintered  $ZrN$ .*
- P. Cristea, et al. LANL *Defect Thermochemistry of Nonstoichiometric Metal Oxides.*
- J. Wallenius, KTH, Sweden, *Atomistic modelling of radiation damage in Fe-Cr alloys.*
- S.G. Srivilliputhur et al. (LANL) *Atomistic Modeling to Develop New Nuclear Fuels: A Case Study Using the Am-N System.*
- S. P. Chen, LANL, *First principles calculations of the transport properties in materials.*
- A. Niklasson, LANL, *Modeling the actinides with disordered local moments.*

**FORMAT:** The first day of the workshop will be dedicated to thermo-mechanical properties and irradiation effects. The second day will start with transport phenomena. A panel discussion on the implications of the modeling and simulations of materials for nuclear fuels and the impact on the fuel performance codes will conclude the workshop. All the presentations will be loaded on a CD and distributed to participants. There will be a 100 USD registration fee. Lunch and refreshments will be provided each day and there will be a sponsored banquet on the evening of the first day, June 9, 2003.

**ABSTRACT SUBMISSION (deadline extended to May 1, 2003):** Please send your abstracts via e-mail to: Marius Stan, Los Alamos Nat. Lab., e-mail: [mastan@lanl.gov](mailto:mastan@lanl.gov), Phone: +1-505-667-8726, Fax: +1-505-667-8021

**REGISTRATION DEADLINE: May 15, 2003.**

**HOTEL registration: May 9, 2003.** There are a limited number of rooms at the downtown *La Fonda Hotel* for the conference price; we encourage the participants to book their rooms as soon as possible.

**ORGANIZING COMMITTEE:** K. Chidester (LANL, Chair), M. Stan (LANL), R. Grimes (Imperial College, London, UK), M. Baskes (LANL), K. McClellan (LANL) and S. P. Chen (LANL)

**Conference coordinator:** Rosemary Romero, Los Alamos National Laboratory, e-mail: [rbromero@lanl.gov](mailto:rbromero@lanl.gov), Phone: +1-505-665-7657, Fax: +1-505-665-4584.

For additional information please visit the workshop web page at: <http://www.lanl.gov/mst/nuclearfuels/>