SUBJECT:	Ph.D. Proposal Presentation
BY:	Narasimhan Swaminathan
TIME:	Friday, June 9, 2006, 3:00 p.m.
LOCATION:	MRDC Building, Room 4211
TITLE:	MECHANICAL-ELECTROCHEMICAL THEORY OF DEFECTS IN IONIC SOLIDS
COMMITTEE:	Dr. Jianmin Qu, Chair (ME) Dr. David L. McDowell (ME) Dr. Meilin Liu (MSE) Dr. Paul A. Kohl (ChBE) Dr. Ting Zhu (ME)

SUMMARY

Mixed ionic electronic conductors (MIEC) have gained tremendous importance recently due to their roles in energy conversion devices such as solid oxide fuel cells, oxygen pumps and gas sensors. Ion and electron transport in MIECs is brought about by a gradient in the electrochemical potential of the defective species. To date, the transport of these defects is generally considered unaffected by the mechanical loading to which the solid is subjected. However, diffusion always takes place under a state of stress due to applied loads, non-uniform thermal or chemical expansion (non-stoichiometry). In this research, the electrochemical potential is derived as a function of the stress state so that the mechanical reliability and the electrochemical performance of the MIEC operating under isothermal steady state condition may be studied under a scenario of stress-diffusion coupling. The stress-dependent electrochemical potential entails the introduction of two material properties, which are the chemical coefficient of expansion (CCE), a second order tensor representing the strains due to non-stoichiometry and a fourth order tensor representing the variation of stiffness with stoichiometry. These properties will be found for common MIECs using molecular dynamics simulation. Finally, the governing differential equations of the coupled problem will be solved using the finite element method. A typical problem involving a plate with a hole (a macro defect in the solid) will be solved using the coupled theory to examine the stress magnitudes and the electrochemical performance of the ionic solid. Conclusions regarding the importance of stress-diffusion coupling and its effects on the mechanical reliability (failure) and electrochemical performance (current, voltage efficiency) will be given for better mathematical modeling of transport and mechanical design of ionic solids for various applications.