THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SPRING COLLOQUIUM SERIES PRESENTS:

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The Kinetic Monte Carlo Algorithm in Materials Science: Study of Radiation-Induced Segregation in Fe-Cr alloys

In this talk I will describe the details of the kinetic Monte Carlo (KMC) algorithm, the theory behind it and its relation with the Markovian master equation. I will then focus on its application to alloy systems under irradiation and how it can model those systems far from equilibrium. Nonequilibrium chemical redistribution in open systems submitted to external forces, such as particle irradiation, leads to changes in the structural properties of the material, potentially driving the system to failure. Such redistribution is controlled by the complex interplay between the production of point defects, atomic transport rates, and the sink character of the microstructure. We have recently developed an interaction model for the Fe-Cr system that incorporates physically accurate thermodynamic driving forces and kinetic coefficients. We have employed this model to analyze the afore-mentioned interplay between alloying elements and irradiation-created defects to study the effect of ideal defect sinks on Cr concentration profiles, with a particular focus on the role of interface density. We observe that the amount of segregation decreases linearly with decreasing interface spacing. Within the framework of the thermodynamics of irreversible processes, a general analytical model is derived and assessed against the KMC simulations to elucidate the structure-property relationship of this system. Interestingly, in the kinetic regime where elimination of point defects at sinks is dominant over bulk recombination, the solute segregation does not directly depend on the dose rate but only on the density of sinks. This model provides new insight into the design of microstructures that mitigate chemical redistribution and improve radiation tolerance.

Dr. Enrique Martinez Saez is a staff scientist at the Los Alamos National Laboratory (LANL), in the Theoretical division. He is the team lead expert on Monte Carlo and Dislocation Dynamics methods applied to materials science and heavily involved in atomistic approaches. Prior to Dr. Saez's current position at LANL, he worked at the Madrid Institute for Advanced Studies of Materials (IMDEA) as a Junior Researcher. Dr. Saez's research interests lie on the study of the microstructural evolution of materials under extreme conditions of irradiation, temperature and deformation and its relation to the macroscopic system response. The design of advanced materials is crucial in the quest for cleaner, more efficient energy sources. Theoretical developments along with modeling and simulation strategies, which Dr. Saez devotes his research to, have become paramount in this quest, to guide and interpret experimental approaches.

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