

Institute for Materials Science

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IMS Rapid Response 2017 * Recipient Guest Seminar



Dr. Frederic Soisson CEA Saclay, SRMP

Kinetics of Segregation and Precipitation in Fe-Cr Alloys Under Irradiation

Thursday, September 14, 2017 10:00 - 11:00 AM MSL Auditorium (TA-03 - Bldg 1698 - Room A103)

Abstract: Fe-Cr alloys are the base of ferritic steels, which are used in a wide range of high-temperature applications. Below 600°C, they undergo a coherent decomposition between Fe-rich (a) and Cr-rich (a') phases, which can be accelerated by irradiation. Irradiation can also lead to radiation induced segregation phenomena, with possible detrimental effects on the material mechanical properties. Segregation and precipitation under irradiation result from a complex interaction between several mechanisms: the acceleration of diffusion due to point defect supersaturation, the annihilation of point defects at sinks, the coupling between the point defects and solute fluxes, the ballistic mixing within displacements cascades. We present an atomic scale modeling of phase separation in Fe-Cr alloys, using ab initio calculations and kinetic Monte Carlo simulations, which take into effects these different mechanisms. The model shows that depending on the irradiation conditions, both enrichments and depletions can be expected at grain boundaries. It shows that for moderate dose rates irradiation strongly accelerates the a', but that a' precipitates are dissolved at higher dose rates, in good agreement with recent experimental observations.

Bio: Frédéric Soisson is a researcher at the Physical Metallurgy Laboratory of the CEA Saclay, near Paris. He got his PhD at the Grenoble Institute of Technology in 1993. Since then, he has been interested in the kinetics of solid state phase transformations and in the evolution of microstructures under irradiation. He studies these phenomena by atomic scale modeling, using techniques such as kinetic Monte Carlo and Mean-Field simulations and DFT calculations.

To be in Dr. Soisson's Agenda, to participate in the Early Career Lunch, or for general information contact: Enrique Martinez Saez <u>enriquem@lanl.gov</u> * 606-2149

Hosted by Enrique Martinez Saez

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