ICAMS
INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

Sergei Dudarev

EURATOM/CCFE Fusion Association
Culham Centre for Fusion Energy
Abingdon, Oxfordshire, UK

Monday, June 24, 4:30 p.m. ICAMS seminar room 0.08

The physics and philosophy of models for fusion materials

The engineering challenge associated with the development of fusion power generation stems from the complexity of materials science and engineering solutions required for realizing this power generation option. Comparing the engineering solutions developed so far for fusion and fission, where both modes of power generation offer low levels of carbon emission, with fusion having further advantage of not generating long-lived radioactive waste, we find that designing a fusion power plant requires a significantly more advanced level of knowledge of structural and functional materials than that needed for constructing a fission power plant.

The scientific challenge associated with the development of fusion materials stems from the fact that while the engineering design criteria and constraints imposed by the phenomena of radiation swelling, hardening, embrittlement, thermal and irradiation creep, and the high temperature loss of strength are all macroscopic, they all are fundamentally related to microscopic events of formation, migration, and interaction between radiation defects and dislocations.

This highlights the pivotal role of the atomic scale in the hierarchy of mathematical modelling methods, involving electronic-, magnetic-, atomistic-, mesoscopic- (Langevin and Monte Carlo) and dislocation-dynamics-based approaches. For example, density functional theory models developed over the last decade have provided unique means for investigating the structure of nano-scale defects produced by irradiation, and for identifying the pathways of migration and interaction between radiation defects. These models, involving no experimental input parameters, are now proving to be as quantitatively accurate and informative as the most advanced experimental observations, creating a new paradigm for the scientific investigation of radiation damage phenomena.

This presentation outlines a range of outstanding questions in the field of radiation stability of iron-based alloys and steels that have recently been addressed and partially resolved using new mathematical concepts and algorithms, validated by dedicated experiments. It also highlights a range of issues specific to fusion power generation technology, including the need to mitigate the effect of neutron-induced transmutation of materials.

This work was funded by the RCUK Energy Programme under grant EP/I501045 and the European Communities under the contract of Association between EURATOM and CCFE. The views and opinions expressed herein do not necessarily reflect those of the European Commission.