

The computational principles of a virtual tokamak reactor

S L Dudarev

UK Atomic Energy Authority, Oxfordshire, UK

The progress of virtual engineering creates a context for the exploration of advanced computer models for materials, to enable the assessment of their performance in a variety of operating conditions. We examine the fundamental principles and applications of self-consistent multiscale materials modelling aiming at predicting the gradual evolution of deformations and stresses at the reactor component scale, stemming from the continuous exposure of a reactor structure to neutron irradiation – which is fundamentally an nuclear and atomic scale microscopic phenomenon. The topics addressed in the presentation include the eigenstrain method for evaluating macroscopic deformations from the density of microscopic defect volume tensors, which can now be derived from ab initio simulations, including density functional theory. We shall also review dynamic atomic-scale simulation algorithms for treating non-linear high dose effects, the power law statistics of defects, and the recent dedicated experimental observations of complex evolving defect microstructures.