VIENNA COMPUTATIONAL MATERIALS LABORATORY

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Can materials modelling assist fusion reactor design?

A talk by Sergei L. Dudarev

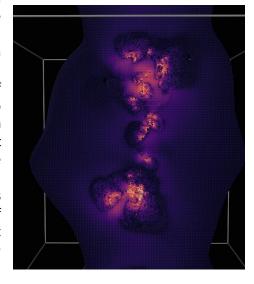
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Neutrons and charged particles produced by nuclear reactions in the fuel assembly of a fission power plant or in the deuterium-tritium plasma of a fusion tokamak produce significant changes in the physical and mechanical properties of materials. These changes result from processes occurring at atomic scale. Fast neutrons initiate collision cascades, in which radiation defects are formed. These

collision cascade events do not change the chemical composition of reactor materials and result only in the formation of fairly stable and relatively well localized distortions of atomic structure; these are the radiation defects. The defects migrate, react, coalesce, and grow, resulting in the formation of a particular type of microstructure, occurring only in materials exposed to irradiation. If the kinetic energy of neutrons exceeds a certain threshold, nuclear transmutations may also occur. In contrast to collision cascades, transmutation reactions modify the chemical composition of irradiated materials. For example, initially chemically pure tungsten bombarded by neutrons transmutes into an alloy containing significant amounts of rhenium, osmium, and tantalum. Transmutations also result in the accumulation of helium and other noble gases in the lattice, stimulating swelling and giving rise to embrittlement.



Quantifying the effects of irradiation on materials requires developing multiscale models for microstructural evolution, which describe how the defects evolve and interact, and how the resulting microstructure responds to external mechanical stress, magnetic fields or temperature gradients. The key parameters defining the response of irradiated materials to macroscopic engineering variables are the operating temperature, irradiation dose and irradiation dose rate. I shall review information about the various properties of candidate fusion materials in the context of fusion reactor design effort, and in relation to the on-going development of models for defect and dislocation microstructure derived from *ab initio* based atomistic and mesoscopic simulations.

