§6. Modeling of Irradiation Performance and Fundamental Data for Fusion Materials

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The basic concept of this task is to integrate theory, modeling and experimental database toward a common focus on a specific technological problem in fusion materials research. IFFS-VI is a program of theory, modeling, simulation and experiments focused on the specific problem of understanding and predicting the effects of temperature variation during fission reactor irradiation on the microstructure development and property changes of V-4Cr-4Ti. This program was devised of the JUPITER collaboration as a means of focusing individual and joint efforts by Japanese and US researchers. The problem chosen aims at the prime candidate material that has received the least attention in that regard so far, but it does not preclude advancements in the general fundamental understanding of irradiation effects. The temperature variation irradiation experiments are currently underway in HFIR. Separate low-dose irradiations will be performed in the JMTR reactor and with heavy ions. They provide experimental information on defect accumulation and property changes under well-controlled and monitored conditions. The temperature variation experiments will also provide a good comparative database against which to evaluate the theories and models in V alloys. V-4Cr-4Ti, other V alloys of interest and some pure metals are among the materials included in the experiments.

This theory and modeling tasks fall into the broad categories of 1)Interatomic Potentials, 2)Defect Properties, 3)Cascade Generation, 4)Annealing Simulation and 5)Comparison with Experiments. It is also pointed out to have a separate detailed task on the effect of the transmutans like H and He under neutron irradiation as well as O, C and N effects.

Good progress toward the goal is expected to be made by building on existing models and using the fundamental defect property database that already exist for vanadium. Although a logical sequence of activities toward meeting the goal is discussed, many of the task elements can be worked on simultaneously and at various levels of physical realism until all the pieces fit together with the requisite level of physical reality.

It is expected that many of the ongoing developments in theory and modeling of irradiation effects are directly relevant to this task without being developed specifically for V-4Cr-4Ti or pure V or even bcc metals and alloys, especially developments of models dealing with defect accumulation and microstructure evolution. These models can be developed in a general way and made specific to V-4Cr-4Ti when cascade and defect property information for that material is available from molecular dynamics simulations and also recent progress in first principles calculations.

Basic information that must be established early on includes interatomic potentials for pure V (some cascade simulations have been done using an embedded atom potential, see below) and for the V-impurity and V-4Cr-4Ti alloy element interactions. These potentials should be developed and tested before further atomistic calculations are performed.