§60. Effect of Solute Trapping on Point Defect Agglomeration in Irradiated Metals

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It has been demonstrated that adding a small amount of impurity may significantly modify irradiation induced microstructures, such as void formation and dislocation development, and consequently alter macroscopic property changes in metals and alloys by a number of experimental works. In modified austenitic steels developed for fusion first wall applications, substantial amount of phosphorus is added to stabilize the microstructure. This strategy has been very successful, for example, in JPCA (Japanese prime candidate alloy), phosphorus-modified US-PCA and simple austenitic alloys, in suppressing void swelling and second phase precipitation. In most these work, microstructural stabilization is attributed to the solid solution effect, namely vacancy-trapping at solute atoms, at relatively low temperatures and to precipitation effect at higher temperatures. This work is primarily intended to clarify how the impurity trapping affects the point defect clustering rates and the defect cluster growth rates under a variety of irradiation conditions, in order to provide theoretical background knowledge how to stabilize microstructures in irradiated materials by a minor compositional modification.

Point defect processes and microstructural evolution under irradiation with collision cascade is complex, because of the instantaneous point defect cluster production within cascade regions and the imbalance in freely migrating point defect production rates. It is well known that the vacancies highly concentrated at the core regions of sub-cascade structures collapse into vacancy clusters (cascade vacancy cluster ; CVC). The morphology, production rates, sizes and stability of the CVC are not sufficiently understood, though they have been studied both experimentally and theoretically. In austenitic alloys, CVC are often observed in a form of stacking fault tetrahedra (SFT), which should have fairly long lifetime due to relatively small formation energy. Some computational work also have predicted possible formation of interstitial clusters as faulted loops within regions surrounding sub-cascade cores. This phenomenon is supported by the discrepancy between the experimentally observed loop population and rate theory calculation of clustering rates of freely migrating interstitials exclusively at low temperatures, but have not yet experimentally confirmed. In the first part of this work, the effect of CVC in various configurations on the temperature dependence of point defect flux is discussed. The second part focuses on the effect of vacancy trapping at solute atoms under cascade damage conditions. A theoretical assessment of the effect of solute-vacancy binding energy and initial solute concentration on point defect flux, defect clustering rates and cluster growth rates is attempted. Followings are the conclusions.

(1) A rate theory model of irradiation effects capable of adopting the output from molecular dynamics simulation studies on defect production efficiency and cascade vacancy cluster formation under high energy neutron irradiation was composed.

(2) A comparison of calculated temperature dependence of swelling rate under various cascade vacancy cluster configuration with experimental data suggested that cascade clusters tend to emit vacancies before they relax into relatively stable configurations such as SFT.

(3) Free SIA and vacancy flux are significantly reduced only when substantial amount of traps with fairly large vacancy trapping energy are present. The reduced point defect flux decreases the degree of vacancy supersaturation and consequently reduces swelling. The swelling suppression through this mechanism requires strong traps (E_b=1.0 eV) at sufficiently higher concentration than the trap-free vacancy concentration.

(4) Relatively weak or low density traps may significantly reduce free helium flux and consequently suppress cavity nucleation in dramatic manner.

(5) Swelling suppression by vacancy trapping may possibly be correlated with the evolution of interstitial type dislocation loops during early stages of irradiation.