

11-1 How Does Impurity Diffuse in Irradiated Materials?

– Evaluation of Impurity Segregation by Diffusion Rate Equations Based on the Atomic Migration Mechanism –

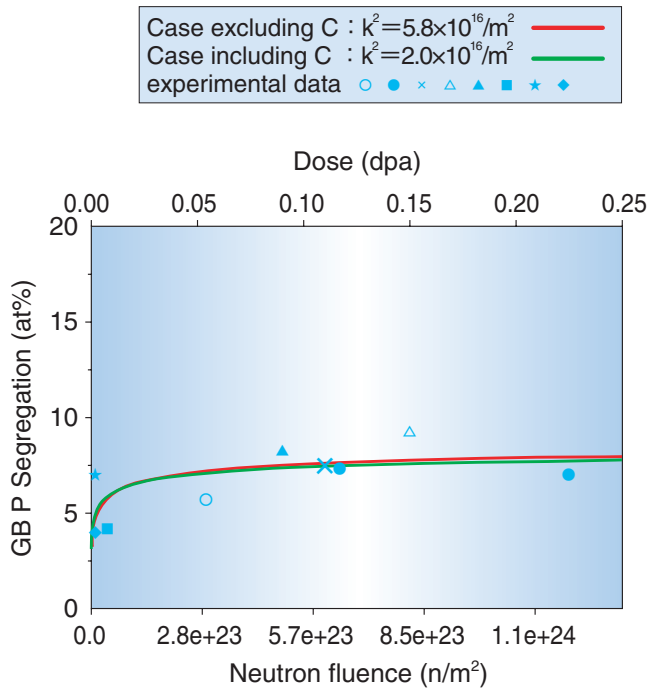


Fig.11-2 GB P segregation vs. dose

The simulation conditions are as follows. P content: 0.013at%, temperature: 290 °C, and dose rate: 1.8×10^{10} dpa/s. The curve of the case including C reproduces the experiments with a sink strength (k^2) lower than that of the case excluding C.

Several impurity elements at grain boundaries (GBs) in steel cause degradation of the toughness of steel by weakening the cohesive strength of the GBs. This phenomenon is known as GB embrittlement. Because irradiation accelerates GB impurity segregation, the evaluation of this segregation in the structural materials of nuclear reactors is an important avenue of research.

Most impurity elements are stable in steel because they are located on crystal lattice points instead of iron atoms. However, when a vacancy (V, a lattice point without any atoms) or self-interstitial dumbbell (SID, formed by two iron atoms that are not on a lattice point) comes to the next lattice point of an impurity atom, the impurity atom can migrate to GBs owing to its interaction with V or SID. As a result, GB impurity segregation is accelerated in irradiated steel, where many Vs and SIDs are generated by the displacement of iron atoms.

We estimated GB segregation of phosphorus (P), which causes GB embrittlement of nuclear reactor pressure vessels, by simultaneously solving diffusion rate equations for V, SID, and P. V and SID decrease when the sink strength in the equations of V and SID is large, such that GB P segregation

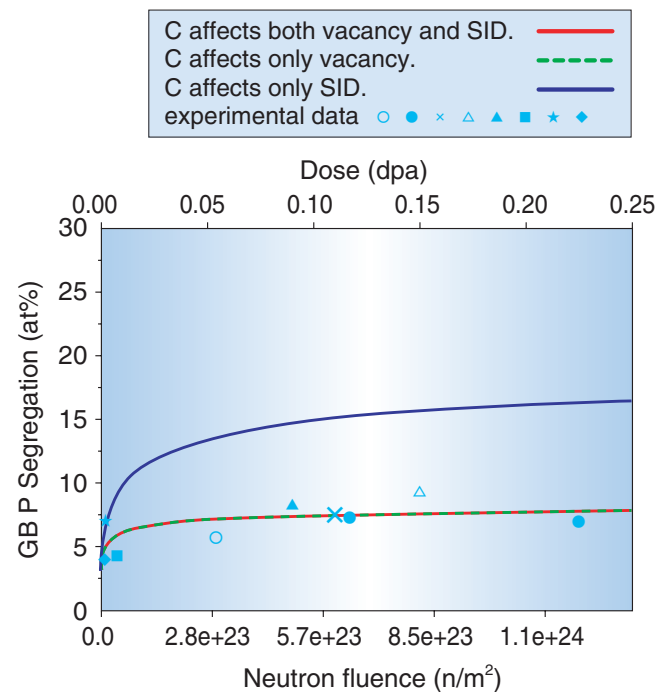


Fig.11-3 Influence of C on GB P segregation

The results for the case where C affects only V are almost the same as those for the case in which C affects both V and SID. Thus, C affects GB P segregation primarily through its effects on V.

is suppressed. While empirical values have been used for the diffusion speeds of V, SID, and P in previous studies, we adopted values that were theoretically derived from several energies and evaluated by atomistic calculation; the energies investigated included the migration energies of V and SID, and the association and dissociation energies between P and V and between P and SID. In addition, because carbon atoms are inevitably included in steel, we estimated the interactions between a V and a C atom and between a SID and a C atom by atomistic calculation and incorporated the effect of C on suppression of diffusion of V and SID into the equations. In the case including C in Fig.11-2, the experimental results were reproduced with a sink strength lower than that in the case excluding C. Thus, we can conclude that C suppresses GB P segregation. We can also conclude that C suppresses GB P segregation primarily through its effects on V (Fig.11-3).

Our method can be applied to GB P segregation of various irradiation conditions and to GB segregation of other diverse impure elements.

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Reference

Ebihara, K. et al., Effect of Carbon on Irradiation-Induced Grain-Boundary Phosphorus Segregation in Reactor Pressure Vessel Steels using First-Principles-Based Rate Theory Model, *Journal of Nuclear Materials*, vol.414, issue 2, 2011, p.328-335.