Interaction of Interstitial Clusters with Solute Atoms in Ferritic Alloys and Its Consequence for Microstructural Development Under Neutron Irradiation

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Up to now the theory of microstructure evolution in irradiated materials has been developed mainly for pure metals. It succeeds in explaining several observations in metals with fcc crystal structure and the difference between swelling under neutron and electron irradiations. The theory emphasises the role clusters of interstitial atoms play in the microstructure development and importance of the steady production of small interstitial clusters directly in displacement cascades under neutron irradiation. Despite this significant success, the understanding of distinguishing features of microstructure development specific to bcc alloys, e.g. low swelling rates, and more generally its sensitivity to material composition is still poor. In this paper, a summary of the information on the interaction of irradiation-produced defects, vacancies and clusters of interstitial atoms, with interstitial carbon, substitutional chromium and copper solute atoms, and copper precipitates in ferritic alloys is presented. This was obtained in recent years from molecular dynamics simulations using existing empirical potentials for the description of interatomic forces and compared with published data from ab initio calculations. It is discussed on the basis of the rate theory that this interaction, especially for interstitial clusters, may be the key for understanding of many features of microstructure development, such as copper precipitate and void growth, under neutron irradiation.

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