Formation of Y-Ti-O nanoclusters in nanostructured ferritic alloys by kinetic Monte Carlo simulations

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Oxide dispersion strengthened (ODS) ferritic alloys are attractive for fusion reactor application because of their improved creep resistance at high temperature. Moreover, a fine dispersion of ODS particle may provide an effective trap for transmutant helium.

We have performed Monte Carlo simulations of the atomic-scale precipitation of Y-Ti-O nanoclusters to understand the precipitation kinetics. The simulation are performed on a rigid body-centered cubic lattice, with oxygen atoms placed on the octahedral sites and Fe, Ti, Y atoms placed on the substitutional sites, following the initial work of Alinger et al. \cite{1}. Thus, two different diffusion mechanisms are involved, oxygen atoms diffusion on the interstitial sublattice and the diffusion of Fe, Ti and Y atoms diffuse by a vacancy mechanism. Extension of the previous work involves introducing a vacancy source and sink to perform kinetic simulations, and an improved assessment of the bonding interaction parameters. In particular, a special site in the simulation box will be devoted to the role of vacancy source and sink, which drives the vacancy concentration toward its equilibrium value. The Fe-Ti-Y-O bonding parameters and saddle point energies will come from thermodynamic and kinetic data on the solubility limits of the different species and phases in alpha-iron, available diffusion coefficients and newly performed ab-initio calculations.

The Monte Carlo results allow us to determine the kinetic path of precipitation, the nature of the nanoclusters with the nucleation of metastable phases, the rate of nucleation and the composition of the nanoclusters as a function of the time. A comparison with experimental results are made.