Atomistic study of hydrogen interaction with intrinsic defects in α-Iron

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The permeation and retention of hydrogen (H) isotopes in materials is a critical issue concerning both economics and safety for realizing controlled nuclear fusion. Reduced activation ferritic/martensitic (RAFM) steel is considered to be the main candidate for the structural material of the future fusion first wall and blanket. In fusion reactors, the radiation of neutrons with 14 MeV high energy will produce irradiation damages (defects), which may exhibit a significant effect on the behavior of H isotopes diffusion, permeation and retention in materials. We chose body-centered-cubic iron (α-Fe) as research object and employed atomistic calculation and simulation methods, including molecular statics calculations, molecular dynamics simulations and genetic algorithm, to study the diffusion properties of H and the interaction between H with different intrinsic defects.

Firstly, we determined that H diffusion in bulk α-Fe as a single atom by molecular statistics calculations. We employed molecular dynamics simulations and obtained H diffusivities, and the effect mechanism of self-interstitial atoms and vacancies on the H diffusion. Further, we studied the distribution and migration mechanism of H atoms around an edge/screw dislocation in α-Fe. Our calculation results reveal that neither edge nor screw dislocations can provide a fast diffusion pipe for H atoms in α-Fe.

Then, we studied the formation mechanism of the vacancy dislocation loop and the interaction between H atoms and dislocation loops in α-Fe. The genetic algorithm was applied to search the energy minimization configuration of vacancy clusters. Molecular statics calculations and dynamics annealing relaxation were employed to calculate the formation and binding energies of vacancies and 3D vacancy or vacancy-hydrogen clusters as well as 2D vacancy or vacancy-hydrogen clusters on {111}, {110} and {211} planes. Our calculations show that vacancies prefer to gather along 3D directions while vacancy-hydrogen clusters prefer to gather along 2D directions, especially on {211} planes. We found that hydrogen atoms are strongly binding by the <100> vacancy dislocation loop and lower the system energy.

Further, we studied the interaction between H atoms and voids. The H atoms trapped by vacancy clusters occupy the octahedral interstitial sites on the surface of the clusters. We obtained the relation between the saturation number of trapped H atoms and the size of vacancy clusters. Further, molecular dynamics simulations were employed to study the behavior of H atoms in voids. H atoms occupy the octahedral interstitial sites on the surface of voids while H molecules exist in voids. As the H number increasing, H molecules in voids atomize and diffuse into the α-Fe lattice, which results in voids collapse.

These calculation and simulation results are of help to understand the diffusion, permeation and retention behavior of H isotopes in RAFM steels as well as the effect of different intrinsic defects. Also, our results can provide important input parameters for larger-scale simulations.