06aC13

Simulation of the behaviors of hydrogen isotopes in tungsten using integrated model

張龍、内村大道、戸田健介、湯山健太、佐藤美咲、大矢恭久、奥野健二
Long Zhang, Hiromichi Uchimura, Kensuke Toda, Kenta Yuyama, Misaki Sato, Yasuhisa Oya and Kenji Okuno

静岡大学大学院理学研究科
Graduate School of Science, Shizuoka University

Tungsten has good thermal and mechanical properties as well as low activation characteristics, which makes it one of the main candidates for fusion reactor plasma facing materials. The interactions between deuterium and tritium with tungsten, which have considerable effects on the safety, reliability, economics aspects, are essential issues for the design and development of nuclear fusion reactors. The out-pile experiments for the behaviors of hydrogen isotopes in tungsten have been carried out extensively. At the same time of the experiments, in order to develop comprehensive simulation tools for reactor design, the modeling for the explanation of these behaviors are indispensable.

The diffusion of hydrogen isotope atoms in tungsten bulk can be modeled by the diffusion equation, $\frac{\partial c_L}{\partial t} = D\nabla^2 c_L$. The main parameter is the diffusivity D, which has Arrhenius relationship with temperatures.

During the diffusion in bulk, the hydrogen isotope atoms might be trapped in various potential wells, including vacancies, dislocations, grain boundaries or defects induced by radiation. These trapping processes can be approximately simulated with the following model:

$$\frac{\partial c_L}{\partial t} = D\nabla^2 c_L - \frac{\partial c_T}{\partial t}$$

$$\frac{\partial c_T}{\partial t} = \nu e^{-\frac{E_D+\Delta E_T}{kT}}\left[c_L\frac{N_T - c_T}{N_L} - e^{-\frac{\Delta E_T}{kT}}c_T\right]$$

The main parameters including the binding energies of hydrogen isotopes in the trapping site, E_T, and the density of trapping sites, N_T.

Since the trapping and de-trapping processes are relatively faster than diffusion process, the local equilibrium of them can be assumed. A simplified model can be obtained:

$$\frac{\partial c_L}{\partial t} = D_{eff}\nabla^2 c_L$$

With:

$$D_{eff} = \frac{D}{1 + \frac{N_T}{N_L}\frac{e^{-\frac{\Delta E_T}{kT}}}{\left(e^{-\frac{\Delta E_T}{kT}} + \frac{c_L}{N_L}\right)^2}}$$

For multi-type of trapping sites, similar terms can be added in the denominator. This simplified model has stability advantages and requires less calculation resources.

Normally, the boundary conditions on the surface of the tungsten can be modeled by the Sievert's law. But in certain situations, for example, plasma-facing materials where the recombination rate of which atoms recombine back into molecules is relatively low, and the implantation rate is high. The recombination flux can be written as: $J = K_r c^2$, where K_r is the surface recombination rate, which depends on the surface conditions of the material. In this situation, the boundary condition is the equilibrium among implantation flux, diffusion flux and recombination flux on surface.

All the above models are integrated together, and an 1-D finite difference method is used for numerical calculation.

Current experiment results are used to validate the model, including:

- Ion-implantation: to validate the boundary condition of surface recombination. The implantation profile is input from other programs like SRIM.
- TDS (Thermal Desorption Spectrum), to validate the diffusion and trapping models.
- Permeation: to validate the diffusion, trapping and surface conditions.