Modeling of hydrogen reactive-diffusive transport and inventory in porous media with mixed materials deposited layers

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Hydrogen isotopes (HIs) retention is a key issue for fusion devices like ITER. Simultaneous use of Be, W and C as the wall material for different parts of plasma-facing components (PFCs) will bring in material mixing issues, which compound that of hydrogen isotopes retention. To simulate the hydrogen inventory in the PFCs, we have developed a flexible standalone model. The particle balance model for reaction-diffusion and hydrogen isotope retention in metal and porous media is presented, respectively. However, in this paper, we only present some basic results based on experimental data available for the purpose of validating the model. More targeted experiments are needed to provide necessary input data for this newly developed model.

I. Introduction

The next-step fusion device ITER can't rely on a single material for plasma facing components. Different materials (Be/W/C) are planned to be used for different parts of ITER [1]. Hydrogen isotope retention is a key issue for designing future fusion reactors, therefore, understanding of the hydrogen isotope inventory processes (HIIPs) in the wall is extremely important; and application of mixed materials in the fusion device makes this even more difficult. Hence a model to simulate the HIIPs is in demand.

A particle balance model for reaction-diffusion and inventory of hydrogen in metals [2] and porous media based on Ref. [3] is presented. At current stage, the model includes three parts: a 1D heating module for the temperature distribution in the wall [4]; a hydrogen metal module for HIIPs in metal materials, and a four region module for hydrogen retention in porous media. The goal of this standalone model is to provide a functional module for present fusion simulation codes (e.g. SOLPS [5]) and to furnish them with a capacity to simulate HIIPs in PFCs. To make the simulations reliable for the HIIPs in different materials, we need a wide variety of experimental data, such as information on trap sites, diffusivity, recombination, grains sizes,

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and wall material compositions, as the input for our code. Hence future targeted experiments for these data are expected.

II. Model

In this section, we will briefly describe the basics of each module.

Heating model

The behavior of HIIPs in the wall is highly dependent on temperature, which plays an important role in hydrogen recycling in a fusion device. We use a heating model for the temporal evolution of the temperature distribution in the bulk, with a heating load $\dot{q}$ at the heating side and a heat sink at the opposite side. Thus, we can write:

$$\rho C_p \frac{\partial T(z,t)}{\partial t} = \frac{\partial}{\partial z}\left(k(T)\frac{\partial T(z,t)}{\partial z}\right) + \dot{q}$$

where ρ and C_p are the density and specific heat of the materials, respectively, and $k(T) = 1/(aT+b)$ is the heat conductivity, where the constants a and b are fitted from experiments [4] .

Using a coolant temperature of $T_0 = 400K$, 1 cm thick walls, and a heat load of $\dot{q} = 3MW/m^2$, we obtain, for Be/W/C materials, the temperature behaviour shown in Fig. 1.

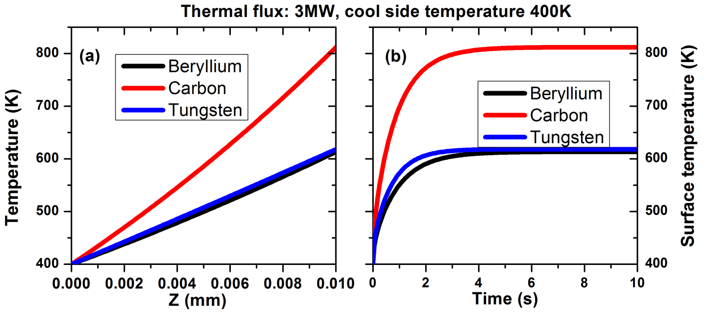

Figure 1: (a) Steady-state temperature distribution inside the wall, (b) time-dependent surface temperature

Hydrogen isotope inventory in metal materials

Beryllium and tungsten are the most important candidates for the first wall of ITER. Four main HIIPs, all thermally activated, are involved in such metal materials: diffusion, trapping, detrapping and surface recombination to form molecules, and can be represented by a set of coupled differential transport equations [2, 6].

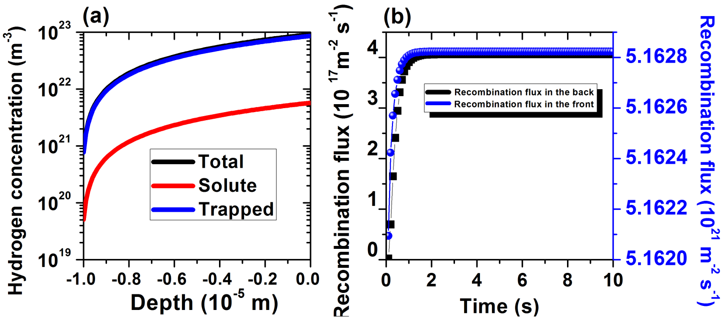

Figure 2: HIIP in Tungsten (a) Hydrogen concentration distribution, (b) time-dependent H_2 recombination flux. Note the variation in scale.

The hydrogen concentration is split into two populations: solute and trapped. In Fig. 2, we present our model results for HIIPs in tungsten, using the following parameters: incoming HIs flux $2 \times 10^{23} m^{-2} s^{-1}$, diffusivity $4.1 \times 10^{-7} e^{-\frac{0.39eV}{kT}}$, recombination coefficient $3.2 \times 10^{-15} e^{-\frac{1.16eV}{kT}}$, intrinsic trap density: 4×10^{-4} (Trap sites / material atoms), the ion-induced traps are not considered. We can see most of the HIs staying inside the wall in traps, and steady-state is reached after a very short time (≈ 2 seconds).

Hydrogen isotope inventory in porous materials

Carbon-based materials and co-deposited layers are made of granules and voids. To simulate HIIPs in porous media, we propose a four-region model: **Region I**, internal surfaces of co-deposit layer; **Region II**, bulk co-deposit; **Region III**, internal surfaces of target material; **Region IV**, Bulk target. (See Fig. 3.) Different regions have distinctive physical processes, which include diffusion, inter-regional transport between surface and bulk (a function of **H**ydrogen **I**sotope **C**oncentration – HIC and diffusivity), Eley-Rideal (ER) processes (a function of incoming flux and HIC) which is surface molecular recombination process, Langmuir-Hinshelwood (LH) processes (a function of HIC^2) which is volume molecular recombination process, **H**ydrogen **D**esorption – HD (an Arrhenius-Boltzmann function of HIC and desorption energy) occuring only in the implantation zone, trapping (a function of HIC and trap site concentration), and detrapping (a function of trapped HIC and the trap energy).

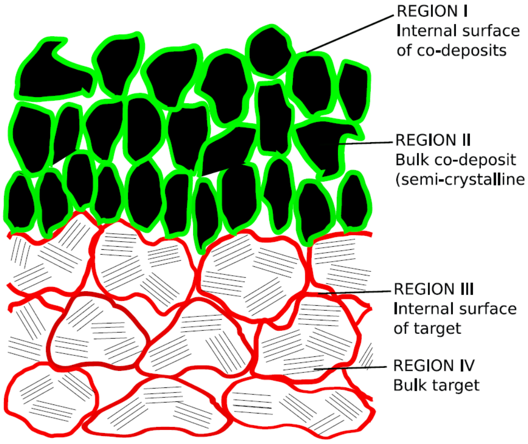

Figure 3: The four regions for plasma facing porous materials

When the HIs particle flux is incident upon the wall, most of the particles will be backscattered, whose rate can be obtained from [7], and a small percentage of them will penetrate the wall, where different reactions happen. For the surface regions (I and III), we consider 7 reactions, which are HD, ER, LH, trapping, detrapping, inter-region transport between surface and bulk, and between bulk and surface. For the bulk regions (II and IV), LH, inter-region transport between surface and bulk, and between bulk and surface are considered.

In this model, the initial trap site concentration is very important to the trapped HICs, however, trap sites produced by particle bombardment are not considered.

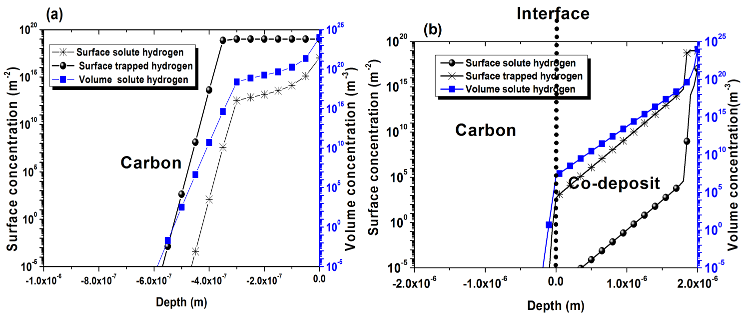

Figure 4: HII (a) two-region for carbon-based target, (b) four region for carbon and co-deposited layer with the interface at z=0.

Figure 4 presents some simple results from a two region (only for carbon) and a four region (carbon and porous co-deposit layer) model. We find a saturated layer where the trap sites are completely occupied (we assume the surface trap concentration is $1 \times 10^{19} m^{-2}$). Below that layer, the HIs diffuse deeper in the co-deposit layer because of its large diffusivity compared the bulk carbon.

Conclusions

A rate model is applied to simulate HIIPs in metal materials and in a four-region description of porous media (including carbon and co-deposit layers), using input from a heating module for the temperature evolution.

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