



Modeling hydrogen isotope behavior in fusion plasma-facing components



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ABSTRACT

In this work, we focus on understanding hydrogen isotope retention in plasma-facing materials in fusion devices. Three common simulation methods are usually used to study this problem that includes Monte Carlo, molecular dynamics, and numerical/analytical methods. A system of partial differential equations describing deuterium behavior in tungsten under various conditions is solved numerically to explain recent data compared to other methods. The developed model of hydrogen retention in metals includes classic, intercrystalline and trapped-induced Gorsky effects. The bombardment and depth profile of 200 eV deuterium in single crystal tungsten are simulated and compared with recent work. The total deuterium retention at various temperatures and fluences are also calculated and compared with available data. The results are in reasonable agreement with data and therefore, this model can be used to estimate deuterium inventory and recovery in future fusion devices.

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1. Introduction

Magnetic fusion energy is a promising next generation source of electricity. The choice of plasma-facing components (PFCs) is a key engineering challenge in fusion reactor design since the interactions between plasma and PFCs are directly related to fuel lost, safety, and wall recovery issues. Carbon, beryllium, and tungsten have been chosen to be the primary materials in the International Thermonuclear Experimental Reactor (ITER). Tungsten has become an essential material in fusion reactor design because of its low erosion yield and high melting point. Therefore, hydrogen isotopes retention and migration in tungsten has transpired into an important safety issue. Consequently, transport and trapping properties of hydrogen isotopes in tungsten is crucial and need further understanding.

Fig. 1 shows a typical hydrogen isotope spatial profile in metal. It is observed in metals such as tungsten [1] which is the focus of this research, as well as stainless steel 304 and 316 [2], molybdenum [3] and Inconel (nickel–chromium based alloy) [2]. Hydrogen isotopes spatial distribution in metal can be generally divided into three regions: near-surface region (I), sub-surface region (II), and bulk (III). The near-surface region has higher concentration due to the incoming hydrogen being implanted and trapped in a few nanometers thickness layer. The sub-surface region shows the classic peak profile of atomic diffusion in metal lattice. In the bulk region, the concentration becomes more flat and slowly decaying and does not change much as hydrogen diffusion extends into the bulk.

In order to explain such spatial profile and the “uphill diffusion” in region II, the classic Gorsky effect is utilized. The Gorsky effect is a diffusion relaxation process first predicted by W.S. Gorsky in 1935 [4], and is observed 30 years later in experiments by Schumann and Alefeld [5] and Cantelli [6]. The Gorsky effect occurs when two conditions are fulfilled: First the point defects need to produce host lattice distortion and change the metal volume, which is true for almost every defect. Secondly, the defect mobility needs to be high enough in order to be observed [6]. Therefore, Gorsky effect is mostly seen in hydrogen–metal systems. For instance, if we bend a beamlike sample, the result would be a stress gradient in the sample and cause interstitial atoms to migrate from the compressive side to the stretching side as schematically shown in Fig. 2.

In 2000, H.R. Sinning first proposed the “intercrystalline Gorsky effect” (IGE) [7,8]. Sinning described IGE as a new relaxation mechanism for hydrogen diffusion in local stress field due to mismatch strain in polycrystalline. Despite the external bending in classical case, the stress gradient is now generated from internal misfits within grains and at grain boundaries. Sinning’s research focuses on measuring dissipation factor and utilizes IGE to explain the broad damping spectrum of hydrogen diffusion in intermetallic compounds. However there is no detail mathematical description of how hydrogen reacts in metal stress field.

As the hydrogen concentration peak shown in region II in Fig. 1, a possible explanation could be that there is a stress field between region I and region II. This stress field ought to be generated from the host lattice distortion by implantation trapped hydrogen in near-surface. Thus, we proposed this stress field as trapped-induced Gorsky effect (TGE). TGE could result in an uphill diffusion

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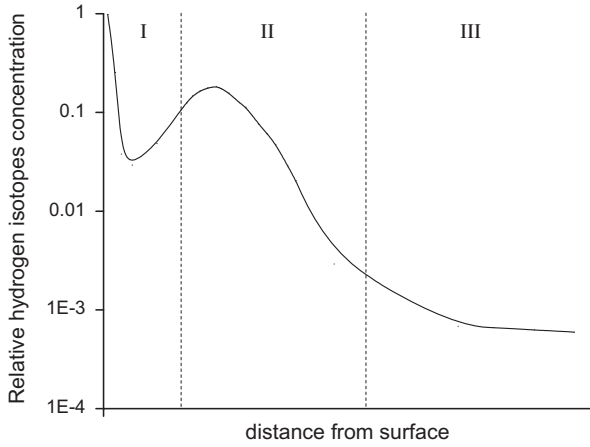


Fig. 1. Hydrogen isotopes depth profile in metal [2].

that is similar to Gorsky effect. The difference is that Gorsky effect depends on external bending stresses while TGE depends on internal lattice distortion. With lattice distortion it would increase the stress and decrease trap sites between region I and region II as illustrated in Fig. 3.

2. Model and methods

2.1. Major equations, ICs and BCs

Most of the traditional diffusion equations solved in this work are the general Fick diffusion equations and boundary conditions developed for the diffuse code described elsewhere [9] which is the first continuum code for hydrogen transport in wall established by M.I. Baskes. The diffuse code utilizes the diffusion equations for solving ion distribution in materials, with numerous conditions and examples such as those given by Wilson et al. [10]. However the pressure gradient is not considered in the common Fick's first law $J = -D \frac{\partial c}{\partial x}$ and second laws $\frac{dc}{dt} = \frac{\partial}{\partial x} (D \frac{\partial c}{\partial x})$ which describe diffusion driven only by concentration gradient. Therefore the diffusion equations need to be modified. We consider the diffusion driven by gradient of chemical potential [11,12]:

$$\mu = \mu^0 + R(\theta - \theta^2) \ln \varphi + p \bar{V}_H$$

where μ^0 is a fixed datum (a standard position or level that measurements are taken from), R is the universal gas constant,

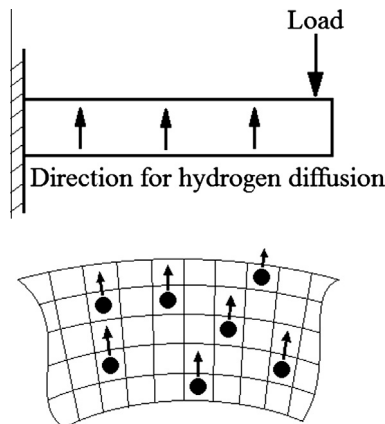


Fig. 2. Migration of interstitial atoms upon sample bending, according to the Gorsky relaxation model [5].

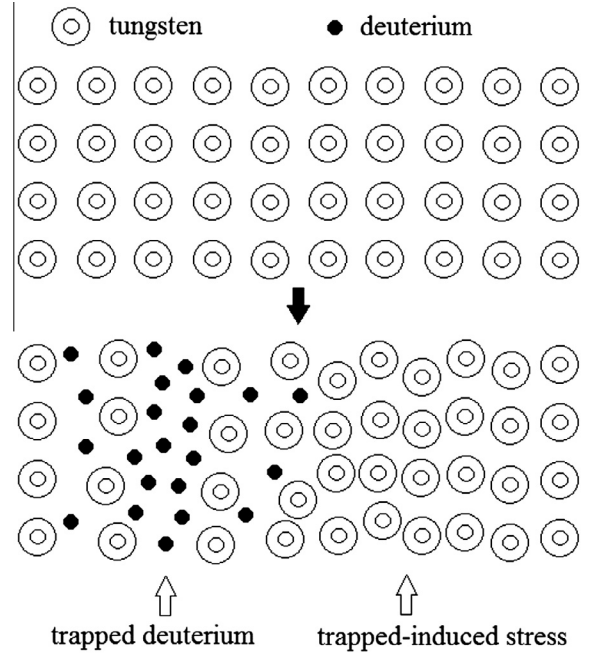


Fig. 3. Possible mechanism of trapped-induced stress.

θ is temperature, θ^2 is temperature at zero Kelvin, φ is normalized concentration defined by $\varphi = c$ (concentration)/ s (solubility), p is the equivalent pressure stress defined as $p = -\text{trace}(\sigma)/3$ and \bar{V}_H is the partial molar volume (the change in volume per mole of hydrogen added to the solid solution). Therefore, the extended flux now includes diffusion driven by temperature and pressure gradients, and is written as [11,12]:

$$J = -sD \left[\frac{\partial \varphi}{\partial x} + \varphi \ln \varphi \frac{\partial}{\partial x} (\ln(\theta - \theta^2)) + \varphi \frac{\bar{V}_H}{R(\theta - \theta^2)} \frac{\partial p}{\partial x} \right] \quad (1)$$

In our work the equations

$$J = -D \left[\frac{\partial c}{\partial x} + c \frac{\bar{V}_H}{R(\theta - \theta^2)} \frac{\partial p}{\partial x} \right] \quad (2)$$

$$\text{and } \frac{dc}{dt} = D \frac{\partial^2 c}{\partial x^2} + \frac{Dc\bar{V}_H}{R(\theta - \theta^2)} \frac{\partial^2 p}{\partial x^2} \quad (3)$$

are used for diffusion induced by concentration and pressure gradients. The general form of p should be calculated from three by three matrix dimension, but since we are doing one-dimensional modeling, and every parameter reduce to degree one in this case, p can simply equals to the pressure value.

The major equations used in the current research for hydrogen isotope behavior in metals can then be written in following:

$$\frac{dc}{dt} = G + D \frac{\partial^2 c}{\partial x^2} + \frac{DC_T \bar{V}_H}{RT} \frac{\partial^2 p}{\partial x^2} - \sum_i \frac{dC_{Ti}}{dt} \quad (4)$$

$$\frac{dC_{Ti}}{dt} = \frac{D}{\lambda^2} C_{\text{Trapi}}^0 \frac{C_{Ti} - C_{Ti}}{W} - C_{Ti} \frac{D_0}{\lambda^2} \exp\left(\frac{-E_{Ti}}{kT}\right) \quad (5)$$

where C is the mobile deuterium atomic concentration; C_T is the total deuterium concentration at that position; C_{Ti} is the i th trapped deuterium atomic concentration; G is the implanted deuterium flux; D is the diffusion coefficient; V_H is the partial molar volume; R is the universal gas constant and p is the equivalent pressure

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