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ABSTRACT:

Hydrogen Diffusion in Samples with Grain Boundaries: How to Account for Traps and Distorted Energy Landscapes

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The transport of hydrogen isotopes within plasma-facing components is crucial for fuel-cycle and safety designs of future fusion reactors. Trap-diffusion modelling is therefore not only of fundamental importance for the analysis of plasma-material interaction experiments (e.g. to extract information about hydrogen isotope trapping energies using thermal effusion spectroscopy) but is also indispensable to estimate tritium retention/permeation in future fusion devices. However, within the last decade the knowledge about adequate modelling assumptions has changed significantly. Firstly, in the light of isotope exchange measurements [1] the standard trapping model had to be changed towards a multilevel trap model [2,3]. Secondly, experimental results have demonstrated that in many circumstances relevant for fusion applications the permeation of hydrogen isotopes in tungsten heavy alloys and recrystallized tungsten samples is dominated by transport along grain boundaries [4]. In that situation main assumptions underlying the McNabb-Foster model [5] (the basis for most trap-diffusion codes used e.g. in fusion research) do not longer hold, e.g. the assumption that the net trapping rate is proportional to the trap concentration. Here we present a parallel finite-volume code RAVETIME which addresses these shortcomings and is capable to simulate transport in inhomogeneous 3-D samples in a consistent way. The computational methodology and performance characteristics (such as weak and strong scalability) of the new code are presented together with first simulation results. These simulation results are compared with experimental data of permeation of hydrogen isotopes through tungsten foils.

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