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On hydrogen transport in solids with traps: influence of broad-band energy distribution and multiple trapping

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Tritium retention in the first wall materials is one of the key issues in the performance of future fusion reactors. Therefore, calculation of hydrogen trapping and transport in fusion wall materials is of particular importance. However, now understanding of underlying physical processes is far from complete. There are experimental phenomena, which are still to be explained, and theoretical predictions, which have not been confirmed or disproved experimentally yet. For example, recent measurements on tokamaks JET and DIII-D showed asymptotic dependence of hydrogen outgassing flux, $\sim 1/t^{0.7}$, instead of expected from classical diffusion $\sim 1/t^{0.5}$. Also, many DFT calculations show that one tungsten vacancy can trap up to 6 hydrogen atoms with different binding energies. This possibility is not usually accounted for in calculations of hydrogen transport, and it is not clear whether it has or not a sufficient influence on the experimental observations.

In the present work we address both of these issues. It was already shown [1,2] that introducing of the broadband distribution of traps over binding energies with hydrogen can explain "anomalous" outgassing flux, mentioned above. Although extension of well-known rate equations, describing hydrogen diffusion in presence of traps, for this case is straightforward, their solution runs into sufficient difficulties. A computer code able to deal with these problems was developed. Modelling of thermodesorption spectra (TDS), performed with the code, demonstrated that the role of additional trap cites can be sufficient in describing experimental results [3].

The model for H transport with multiple trapping was developed. The main equations of the model are a further development of the rate equations for diffusion in presence of traps. These equations are intrinsically nonlinear and their solution in the general case can be obtained by numerical calculations. However, several limiting cases when analytical solution is possible were considered. Analysis of these simple situations gives a general understanding of effect of multiple trapping on H transport. In order to investigate possible influence of multiple trapping on TDS, numerical solution was done.

References

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