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A kinetic model based on DFT for H atoms transport at the W/Cu interface

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This study explores the diffusion of hydrogen (H) across the tungsten (bcc) - copper (hcp) W(001)/Cu(11-20) interface [1-3]. It combines DFT electronic structure calculations and kinetic modeling based on diffusion coefficients and macroscopic rate equations (MRE). The copper lattice reconstructs significantly near the interface, inducing complex energetics for hydrogen atoms inserted at the interface. The many solution energies of hydrogen absorbed in these different interstitial sites have been calculated, as well as the complex hydrogen diffusion energy profile at the interface. Two diffusion paths across the interface were considered, connected by a third path in the plane of the W/Cu interface.

The activation barriers within the copper network displayed significant variations among these paths due to the reconstruction of the Cu fcc bulk into a hcp structure in the vicinity of the interface. Additionally, diffusion properties are established in perfect tungsten and copper as a reference. They are compared to diffusivity across and parallel to the W/Cu interface. Notably, diffusion parallel to the interface is shown to be lower than that within the tungsten and copper bulks across the temperature range from 260K to 1000K. Subsequently, the hydrogen diffusion perpendicular to the interface plane was modeled and analyzed according to a kinetic model we built based on 0-dimension Macroscopic Rate Equations. The complex energy pattern of the diffusion path across the interface behaves like a two steps model. Consequently, a model is proposed to model the kinetic behavior of H transport across the W/Cu interface. This reduced model reproduces the results of the full kinetic model with great accuracy. It also proves robust when the boundary solutions applied to solve the system of differential equations are modified.

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[3] Y. Silva-Solis, J. Denis, E. A. Hodille, Y. Ferro, Nuclear Materials and Energy Fusion, 37 (2023) 101516

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