Ab Initio Simulation Study of Interfaces in Nanostructured Tungsten

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Abstract

In both, inertial and magnetic confinement fusion, reactors, the walls have to withstand high thermal loads and radiation fluxes. This work reports on a first principles study of the light atoms behavior (H , H-isotopes and He) in nanostructured tungsten. In order to carry out this work we present the approximation of the necessary foundations for the analysis using the SIESTA code [1]. The results are compared to data [2-3] obtained with a more precise plane wave code as VASP [4]. Moreover, the work is aimed to interpret experimental results on structural and mechanical properties measured by the Materials group at the Institute of Nuclear Fusion. The obtained results are valuable for subsequent simulations on a larger scale, such as kinetic Monte Carlo [3] or Molecular Dynamics. This complete analysis allows having a nanoscopic view of phenomena leading to bubble formation and eventual trapping of light atoms at vacancies and in the bulk of tungsten, as well as at the interfaces.

References

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