DFT simulations of the behavior of aggregates of light impurity atoms in the presence of intrinsic point defects in a tungsten grain boundary

Jorge Suárez-Recio[1,2,*], Darío Fernández-Pello[1], María Ángeles Cerdeira[1], Raquel González-Arrabal [2], César González [3,4], Roberto Iglesias[1] *

[1]*Departamento de Física, Universidad de Oviedo, E-33007 Oviedo, Spain*

[2]*Instituto de Fusión Nuclear, Departamento de Ingeniería Energética, Universidad Politécnica de Madrid, E -28006 Madrid, Spain*

[3]*Departamento de Física de Materiales, Universidad Complutense de Madrid, E-28040 Madrid, Spain*

[4]*Instituto de Magnetismo Aplicado UCM-ADIF, E-28230 Madrid, Spain*

* Corresponding author: j.srecio@upm.es

Nanostructured materials with multiple grain boundaries showing diverse orientations have shown a great ability to reduce the damage that will be produced by irradiation in a future nuclear fusion reactor [1], being nanostructured tungsten a especially prominent candidate material [2]. Among the diversity of deleterious effects produced by the impact of high energetic particles on first wall or plasma facing materials, the formation and aggregation of vacancies and interstitials and the ubiquitous presence of hydrogen and helium that would eventually end up in bubble formation, in obvious detriment of the performance and operational life of such structural materials, play a major role. To assess the above issues, DFT simulations focused on an energetic, structural and mobility analysis of the effects due to the simultaneous presence of intrinsic (vacancy, self-interstitial atom, SIA) and extrinsic (light impurity atoms, LIA) point defects in a W110/112 grain boundary (GB), appearing because of the impinging radiation in a fusion environment, have been performed.

For that purpose and based on our previous and very recent work [3], aggregates of LIAs have been placed inside or in the vicinity of a vacancy, to find out if a SIA can compete and recombine with the latter or, on the contrary, such recombination is obstructed by the simultaneous presence of helium or hydrogen. In a realistic environment, especially for temperatures at which vacancy mobility is already activated, He could hamper the vacancy-SIA recombination process at the GB which would prevent the self-healing effect.

[1] I. Beyerlein et al, Prog. Mater. Sci. 74 (2015) 125.

[2] R. González-Arrabal et al, J. Nucl. Mater. 453 (2014) 287.

[3] D. Fernández-Pello, et al., J. Nucl. Mater. 560 (2022) 153481.