An Object Kinetic Monte Carlo comparison of helium retention in nanocrystalline tungsten and monocrystalline tungsten

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Abstract

Tungsten is an excellent candidate for plasma facing components (PFC) in future fusion reactors since it offers several advantages: high melting point, high thermal conductivity, low sputtering coefficient and low tritium retention. However, tungsten will be exposed, among other ions, to helium irradiation. Due to helium insolubility in metals, its implantation inside vacancy-like defects leads to He bubble formation and eventually to detrimental exfoliation of the material. Nanostructured tungsten is nowadays under research because of its large grain boundary density: a high fraction of the incoming helium will be retained inside the grain boundaries. As a result of this behavior, the vacancy defects filled with helium atoms in the interior of the grains in nanocrystalline tungsten are expected to be less pressurized than in case of monocrystalline tungsten.

In this work we present OKMC (Object Kinetic MonteCarlo) simulations of helium (625 keV) pulsed irradiation (10^{13} cm^{-2} He/pulse) in both monocrystalline and nanocrystalline tungsten, following the experimental conditions carried out by Renk et al. [1]. The simulator used in this work is MMonCa, a recent developed OKMC code [2]. Nanocrystalline tungsten is formed by columnar grains of 1300 × 50 × 50 nm^3. The surrounding grain boundaries are taken as perfect sinks for all defects (vacancies, SIAs, He atoms and their clusters). Comparing both monocrystalline and nanocrystalline tungsten, a clear role of the grain-boundary density in helium retention in the interior of the grain is observed: the higher the density the lower the He retention, that is, the lower the amount of He atoms inside vacancy-like defects. Also can be seen a difference in the He-V defects configuration: our results show that nanocrystalline tungsten exhibits a clear reduction in the number of undesired pressurized He-V clusters as compared to monocrystalline W. The parameterization of MMonCa code for He in W is based on previously published data [3,4] and has been tested comparing to experimental results [5].

References

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