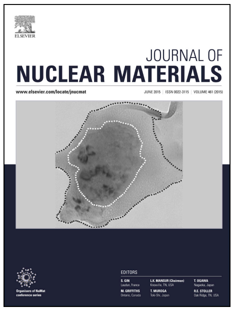

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On the onset of void swelling in pure tungsten under neutron irradiation: an object kinetic Monte Carlo approach

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Abstract

We propose an object kinetic Monte Carlo (OKMC) model for describing the microstructural evolution in pure tungsten under neutron irradiation. We here focus on low doses (under 1 dpa), and we neglect transmutation in first approximation. The emphasis is mainly centred on an adequate description of neutron irradiation, the subsequent introduction of primary defects, and their thermal diffusion properties. Besides grain boundaries and the dislocation network, our model includes the contribution of carbon impurities, which are shown to have a strong influence on the onset of void swelling. Our parametric study analyses the quality of our model in detail, and confronts its predictions with experimental microstructural observations with satisfactory agreement. We highlight the importance for an accurate determination of the dissolved carbon content in the tungsten matrix, and we advocate for accurate description of atomic collision cascades, in light of the sensitivity of our results with respect to correlated recombination.

Keywords:
Tungsten, Kinetic Monte Carlo, Neutron Irradiation, Void Swelling

1. Introduction

Tungsten is currently the officially selected constituent material for the divertor in ITER, and also for the first wall armour in the DEMO project [1, 2, 3]. This choice is mainly guided by its high melting point, high strength and high resistance to sputtering. In these reactors, the plasma-facing material is foreseen to experience extreme conditions, including a high heat load (up to 20 MW m^{-2} in normal conditions), a high flux of bombarding plasma particles (over $10^{24} m^{-2} s^{-1}$) and, also, a high flux of fast neutrons emitted from the fusion reactions [4]. In spite of the above-mentioned advantageous interaction properties with plasma, however, the intrinsic brittleness of tungsten can be regarded as the major safety issue, in particular for concepts including water-cooled divertors [5]. Even non-irradiated tungsten, for instance, is characterized with a ductile-to-brittle transition temperature (DBTT) as high as $300 - 400°C$ [6]. While this transition appears to be originally determined by the thermal activation of screw dislocations, neutron irradiation continuously generates lattice defects that further obstruct their glide, thus shifting the DBTT to even higher values. In any case, operation below DBTT induces a risk of cracking for plasma-facing components, because they cannot dissipate thermal stresses by plastic deformation [7]. If plasma damage is associated to a rather narrow penetration depth (around a few tens of micrometers as revealed by direct TEM investigations [8, 9]), neutron irradiation, in contrast, affects the whole components resulting in a nearly homogeneous damage rate; the consequent microstructure pattern should, nevertheless, be strongly heterogeneous because of the temperature gradient from the plasma-facing surface towards heat sinks [10]. Undoubtedly, the present lack of consistent data on the performance of tungsten with respect to heat loads and transients under neutron irradiation remains to be filled in.

Accurate knowledge and understanding of the microstructural evolution of tungsten under neutron irradiation is an essential pre-requisite to rationalize and predict the resulting changes in its mechanical properties. For these reasons, such investigations are nowadays a "hot topic" in the field of fusion material development [11, 12]. In substitute to full-scale fusion material testing facilities, experimental studies are conducted with fission test reactors [13, 14, 15, 16, 17] in spite of the intrinsic differences in the neutron spectra involved. To start with, the thermal-to-fast neutrons ratio is, naturally, much higher in fission reactors, with consequences on the rate of transmutation to rhenium or osmium. Secondly, because of the presence of 14 MeV neutrons, the transfers of kinetic energy from impinging neutrons to primary knock-on atoms, with subsequent occurrence of atomic collision cascades, largely differ between fission and fusion reactors. This has a significant impact on the primary production of damage, and thus also potentially on the long-term evolution of the microstructure, as discussed later in section 2.3. Undoubtedly, these discrepancies in experimental set-ups, and therefore the underlying questions of transferability of experimental evidences from fission to fusion environments, imply a need for complementary computer-based modelling activities, where the design-relevant informations about the neutron spectrum and transmutation rates are adequately embedded.

Experimental evidence [16, 17, 18] highlights that the mi-

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