Accepted Manuscript

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PII: S0022-3115(17)31341-7

DOI: 10.1016/j.jnucmat.2018.01.059

Reference: NUMA 50767

To appear in: *Journal of Nuclear Materials*

Received Date: 24 September 2017

Revised Date: 6 January 2018

Accepted Date: 30 January 2018

Please cite this article as: Y. Chen, Y.-H. Li, N. Gao, H.-B. Zhou, W. Hu, G.-H. Lu, F. Gao, H. Deng, New interatomic potentials of W, Re and W-Re alloy for radiation defects, *Journal of Nuclear Materials* (2018), doi: 10.1016/j.jnucmat.2018.01.059.

New interatomic potentials of W, Re and W-Re alloy for radiation defects

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Abstract:

Tungsten (W) and W-based alloys have been considered as promising candidates for plasma-facing materials (PFMs) in future fusion reactors. The formation of rhenium (Re)-rich clusters and intermetallic phases due to high energy neutron irradiation and transmutations significantly induces the hardening and embrittlement of W. In order to better understand these phenomena, in the present work, new interatomic potentials of W-W, Re-Re and W-Re, suitable for description of radiation defects in such alloys, have been developed. The fitted potentials not only reproduce the results of the formation energy, binding energy and migration energy of various radiation defects and the physical properties from the extended database obtained from DFT calculations, but also predict well the relative stability of different interstitial dislocation loops in W, as reported in experiments. These potentials are applicable for describing the evolution of defects in W and W-Re alloys, thus providing a possibility for the detailed understanding of the precipitation mechanism of Re in W under irradiation.

Keywords

W-Re alloy; Empirical potentials; Radiation defects; Molecular dynamics simulation

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