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FIRST-PRINCIPLES MODELLING OF ANOMALOUS PRECIPITATION IN NEUTRON-IRRADIATED W(RE,OS) ALLOYS

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Segregation occurring in under-saturated solid solutions under irradiation is a mysterious phenomenon that potentially has significant practical implications [1,2]. In this study, a new multi-scale modelling approach, based on first-principles calculations, is developed, where solute atoms (Re, Os) and vacancies (Vac) are treated as components of a quaternary alloy. The free energy of W-Re-Os-Vac alloys is evaluated as a function of temperature and vacancy concentration using effective CE interactions and quasi-canonical Monte Carlo (MC) simulations. In the low solute concentration range (< 5 at%Re), our simulations predict the formation of precipitates with Re concentration that agrees with experimental observations of self-ion irradiated W-1at.% Re-1at% Os alloys. Quenched MC predictions for W-1.5% Re-0.25%Os alloys simulated at T=1200K show that precipitates may adopt the form of (110) faceted voids with surfaces enriched by Re atoms, with the average concentration of Re close to 14%. This agrees well with recent Transmission Electron Microscopy observations of neutron-irradiated W samples [2]. Strong Os-vacancy cluster interactions predicted by ab-initio calculations play a crucial role as a precursor of anomalous radiation-induced precipitation occurring in dilute W alloys [3].

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[3] J. S. Wrobel, D. Nguyen-Manh, K.J. Kurzydlowski, S.L. Dudarev, J. Phys. : Condensed Mater. **29** (2017) 145403.

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