Design of efficient interface-controlled self-healing from radiation damage: DFT simulations of He bubble formation and migration processes in metals

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Abstract

Recently, interfaces between incoherent transition metal nanolayers showing semicoherent heterophase structures and lattice parameter mismatches have been proposed as perfect sinks for absorption of radiation-induced defects at intersections between misfit dislocations [1]. An accurate description from first principles of the diverse types of point defects in irradiated metals appears as an essential preliminary step towards the design of efficient multilayered materials capable of self-healing from radiation damage. Among such defects, helium appears as a by-product of transmutation reactions taking place in the structural materials inside future fusion reactors. He tends to form clusters that are trapped within vacancies and ultimately coalesce as gas bubbles that cause swelling and embrittlement, severely deteriorating the integrity, toughness and overall performance of the material. Hopefully, it is expected to accumulate at the appropriately designed multilayered interfaces from where it can scape or be extracted afterwards. Consequently, a systematic energetic and structural study of the formation and mobility of small clusters of vacancies and He atoms in the bulk of several transition metals, namely, Cu, W, and Nb, that have been identified as possible candidates for building these interfaces has been performed. Our results show that migration energies are lower when the vacancy clusters do not contain He atoms [2], suggesting that He trapping is a highly efficient mechanism of stabilisation and eventual immobilisation of vacancies, so reducing the severe embrittlement via bubble formation [3].

References

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