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Self-healing mechanism of irradiation defects in nickel–graphene nanocomposite: An energetic and kinetic perspective

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Abstract: The self-healing mechanism of radiation-induced defects in nickel–graphene nanocomposite is investigated by atomistic simulations. Compared with pure nickel, nickel–graphene nanocomposite has less defects remained in the bulk region after collision cascades, illustrating self-healing performance. Nickel–graphene interfaces (NGIs) serve as sinks for radiation-induced defects and preferentially trap interstitials over vacancies. Energetic and kinetic calculations reveal that the defect formation energy and diffusion barrier are reduced in the vicinity of NGIs, and the reduction are pronounced for interstitials. When NGIs are loaded with interstitials, their segregation ability on radiation-induced defects improves significantly, and the radiation-induced defects near the NGIs diffuse more easily. Especially, the vacancies (or interstitials) near the NGIs tend to annihilate (or aggregate) with the interstitials trapped at the NGIs, which only happens at the interstitial-loaded side of NGIs. Therefore, nickel–graphene nanocomposite exhibits excellent radiation tolerance and shows promise as a structural material for advanced nuclear reactors due to its NGIs with the energetic and kinetic driving forces acting on radiation-induced defects.

Keywords: Nickel–graphene nanocomposite; interfaces; irradiation defects; self-healing; atomistic simulations

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