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Iodine atom diffusion in SiC and Zr

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Silicon carbide (SiC) is a promising cladding material in light water reactor. The fuel cladding is an important safety barrier in fission nuclear reactors, as it restrains most of the radioactive fission products within its volume. The ability to keep radioactive fission products within the cladding material determines whether SiC can be used as a safe cladding material. Iodine atom diffusion in SiC is calculated with first-principles calculation and nudged elastic band method (NEB) and compared with that in Zr. Without considering vacancy effect, the diffusion rate of iodine in SiC is slower than that in Zr. Consider the vacancy from the neutron irradiation, divacancy can speed up iodine impurity diffusion in SiC. Even larger vacancies slow down iodine diffusion in SiC. Meanwhile, vacancies slow down the diffusion of iodine atom in Zr.

Biography

Wei Xiao has completed his PhD from University of California, Berkeley. He is a Senior Scientist and a Team Leader of nuclear materials simulation group at State Nuclear Power Research Institute, China.

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