Corresponding Author

Benjamin Beeler

North Carolina State University

[bwbeeler@ncsu.edu](mailto:bwbeeler@ncsu.edu)

Dear Editorial Board,

Journal of Nuclear Materials

In this study, we present a density functional theory (DFT) investigation of the diffusion behavior of lanthanide and actinide solutes—specifically cerium (Ce), neodymium (Nd), uranium (U), and plutonium (Pu)—in body-centered cubic (BCC) iron (Fe). Fuel-cladding chemical interaction (FCCI) is a key degradation mechanism in sodium-cooled fast reactors, driven by the migration of fission products and fuel constituents into Fe-based cladding. To elucidate this process, we combined DFT with self-consistent mean field (SCMF) theory to calculate vacancy-mediated diffusion coefficients for these solutes both in bulk BCC Fe and, for the first time, on the (110) surface.

In bulk BCC Fe, Ce, Nd, U, and Pu diffuse substantially faster than Fe self-diffusion despite high migration barriers, due to strong vacancy drag effects for these oversized solutes. At high temperatures (T = 1000 K), solutes diffuse 2–3 orders of magnitude faster than Fe, increasing to 4–8 orders at low temperatures (T = 500 K). Surface diffusion is significantly faster than bulk, with activation energies reduced by 0.7–0.9 eV. The calculated surface diffusivities show similar temperature dependence to experimental grain boundary (GB) diffusivities in the literature. For oversized solutes, we propose that vacancy-mediated diffusion is the dominant transport mechanism along GBs, indicating that the computed surface diffusivities provide reasonable estimates for lanthanide and actinide migration along GBs in Fe-based cladding.

These findings provide new insights into the atomic-scale mechanisms governing FCCI in Fe-based cladding and offer critical inputs for higher-length scale modeling of cladding degradation in advanced reactors.

Sincerely,

Benjamin Beeler