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Dear Editorial Board,

Journal of Nuclear Materials

On behalf of my co-authors and myself, I am hereby submitting our manuscript, entitled “*First-Principles Investigation of Cerium and Neodymium Diffusion in BCC Chromium and Vanadium via Vacancy-Mediated Transport”* to your journal.

In this study, we present a density functional theory (DFT) investigation of the diffusion behavior of lanthanide fission products—specifically cerium (Ce) and neodymium (Nd)—in body-centered cubic (BCC) chromium (Cr) and vanadium (V). Fuel-cladding chemical interaction (FCCI) is a well-known contributor to fuel pin failure in sodium-cooled fast reactors. A promising mitigation strategy involves introducing interdiffusion barriers, such as Cr coatings or V liners, between the fuel and cladding. However, the efficacy of these materials in limiting the diffusion of lanthanide fission products has not been thoroughly explored. Using DFT in combination with self-consistent mean field (SCMF) theory, we computed vacancy-mediated diffusion coefficients for Ce and Nd in BCC Cr and V. Our results show that both Ce and Nd behave as oversized solutes, forming strong bonds with vacancies and occupying off-lattice positions. The calculated diffusivities and segregation tendencies are compared to those in hexagonal close-packed (HCP) Zr, previously studied by our group. We find that lanthanide diffusion in Cr is significantly slower than in Zr, whereas diffusivities in V are comparable to those in Zr. Despite these lower equilibrium diffusivities, both Cr and V exhibit strong vacancy drag effects and a pronounced tendency for solute enrichment at vacancy sinks. Under irradiation, this behavior may promote lanthanide migration toward interfaces, potentially intensifying FCCI at the liner–cladding boundary.

We believe our findings provide new insights into the selection and optimization of liner materials for mitigating FCCI in advanced reactors. The diffusion data and analysis presented in this work may also serve as input for higher-scale models such as rate theory, cluster dynamics, and phase-field simulations.

Sincerely,

Benjamin Beeler