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First-principles investigation of boron incorporation into CRUD under Pressurized Water Reactor conditions ZS. RAK, C.J. O'BRIEN, D.W. BRENNER, Department of Materials Science and Engineering, North Carolina State University — CRUD (Chalk River Unidentified Deposit) is predominately a nickel-ferrite deposit on hot surfaces of nuclear fuel rods during reactor operation. The presence of CRUD modifies the core-coolant heat transfer and can induce localized corrosion on the cladding surface. Besides these unwanted effects boron, which is a neutron absorber, can accumulate within the CRUD, triggering shifts in the neutron flux and fluctuations in the reactor power level. Therefore, it is crucial to understand and predict the mechanisms by which B is trapped into the CRUD. As a first step, the incorporation of B defect into the crystal structure of $NiFe_2O_4$ has been investigated using the DFT framework. To obtain the formation energies of various interstitial and substitutional B-defects, theoretical results have been combined with experimental thermo-chemical data. Assuming solid-solid equilibrium conditions, the main factors that limit the incorporation of B are (i) the narrow stability domain of the host $NiFe_2O_4$ and (ii) the formation of ternary Fe-B-O and Ni-B-O compounds. The study also investigates the incorporation of B assuming solid-liquid equilibrium between $NiFe_2O_4$ and the surrounding aqueous solution under conditions of pressure, temperature, and pH characteristic to pressurized water reactors.

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