

Computational Studies of Grain Boundary Behavior in Uranium Dioxide Nuclear Fuels

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Nuclear power is responsible for the production of 380,000 Megawatts of energy worldwide, which results in over 11% of the world's energy production [world-nuclear.org]. Pellet-cladding interactions (PCI) are a key nuclear fuel failure mechanism which presents formidable challenges to researchers due to extreme nuclear fission conditions. Although PCI interactions have been reduced due to fuel additives, understandings of PCI interactions remain elusive. We propose new approaches to increase understanding of nuclear fuel interactions; specifically, uranium dioxide and the effects of dopants. This study focuses on amorphous uranium dioxide and fission products, while benchmarking new methods with previous computational studies. Results will further research into modeling approaches and help guide future experimental design.

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