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Molecular dynamics modeling of radiation damage in Ni-Fe concentrated alloys

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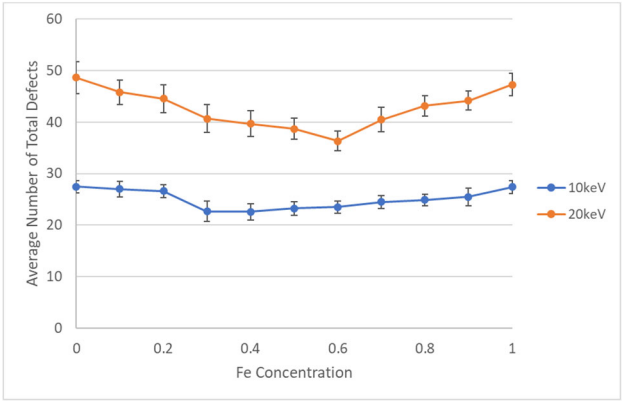
Abstract

Nuclear energy makes up a significant portion of clean energy production, offering many advantages over other clean energy sources. Materials play a significant role in the safety of nuclear energy. Radiation damage causes the degradation of many material properties including mechanical properties, due to the evolution of supersaturated defects created by radiation. The development of radiation tolerant materials is critical to ensuring safety and long operational life. Concentrated alloys show promise as reactor materials because of their improved radiation performance compared with conventional dilute alloys. In this study, Molecular Dynamics simulations are performed on a wide range of Ni-Fe concentrated alloys to examine their defect production behavior. The Ni-Fe alloy composition ranges from pure Ni to pure Fe, in increments of 10 at.% Fe. The initial alloy structures are optimized with the Metropolis Monte-Carlo method to ensure each alloy has good mixing. These alloys are then subjected to a simulated radiation cascade, where an atom is imparted energy as if hit by a radiation particle. The final defect structures after primary damage are analyzed with different defect characterization methods to obtain the surviving defect statistics. It is found that defect production is minimized around Ni-50%Fe, indicating that concentrated alloys do suppress defect production under irradiation, which is consistent with experimental observations.



The average number of total defects after primary damage in Ni-Fe concentrated alloys as a function of Fe concentration.

Biography

My name is Jason Brown, and I am pursing an M.Eng. degree with an expected completion date of 05/13/21. I started my degree in 2018 as an undergraduate and have been a part-time remote student while working full time since 2019. I am in Dr. Bai's research group, and I am investigating the effect of concentrated alloys on defect production behavior under irradiation.