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Molecular Dynamics Simulation of Irradiation-Induced Damage Cascades in Graphite

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Abstract : Graphite is the matrix, and structural material in the high temperature gas-cooled reactor exhibits an irradiation response. It is of significant importance to analyze the defect production and evaluate the role of graphite under irradiation. A vast experimental literature exists for graphite on the dimensional change, mechanical properties, and thermal behavior. However, simulations have not been applied to the atomistic perspective. Remarkably few molecular dynamics simulations have been performed to study the irradiation response in graphite. In this paper, irradiation-induced damage cascades in graphite were investigated with molecular dynamics simulation. Statistical results of the graphite defects were obtained by sampling a wide energy range (1–30 KeV) and 10 different runs for every cascade simulation with different random number generator seeds to the velocity scaling thermostat function. The chemical bonding in carbon was described using the adaptive intermolecular reactive empirical bond-order potential (AIREBO) potential coupled with the standard Ziegler–Biersack–Littmack (ZBL) potential to describe close-range pair interactions. This study focused on analyzing the number of defects, the final cascade morphology and the distribution of defect clusters in space, the length-scale cascade properties such as the cascade length and the range of primary knock-on atom (PKA), and graphite mechanical properties' variation. It can be concluded that the number of surviving Frenkel pairs increased remarkably with the increasing initial PKA energy but did not exhibit a thermal spike at slightly lower energies in this paper. The PKA range and cascade length approximately linearly with energy which indicated that increasing the PKA initial energy will come at expensive computation cost such as 30KeV in this study. The cascade morphology and the distribution of defect clusters in space mainly related to the PKA energy meanwhile the temperature effect was relatively negligible. The simulations are in agreement with known experimental results and the Kinchin-Pease model, which can help to understand the graphite damage cascades and lifetime span under irradiation and provide a direction to the designs of these kinds of structural materials in the future reactors.

Keywords : graphite damage cascade, molecular dynamics, cascade morphology, cascade distribution
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