Evolution of Threshold Displacement Energy in Irradiated Graphite

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Graphite plays a vital role in current and future (GenIV) nuclear fission reactor designs, often serving as both a structural component and neutron moderator. Elucidating the effects of neutron irradiation in graphite is therefore key in furthering future reactor design and informing the decommissioning of current reactors. Whilst defects in pristine graphite and their formation processes are well understood, recent work has shown that the structure and texture of graphite changes when irradiated[1;2], thus altering the physical properties of the material. The threshold displacement energy ($\mathbf{E_d}$) of a material is the minimum energy required to create a defect, with a value of 60 eV currently used as the accepted industry standard for nuclear-grade graphite[3].

In this work, molecular dynamics simulation is used to study the evolution of threshold displacement energy in irradiated graphite with damage ranging from zero to one displacement per atom. A large number of initial primary knock-on atom directions sampling energies from 5 to 100 eV are used to ensure statistically significant results. A defect creation criterion is generalised for non-crystalline carbon and is found to produce equivalent results when compared to existing definitions in pristine graphite. The time-dependent image guided atomistic reconstruction (IGAR)[4] models of irradiated graphite are used with interactions treated using the carbon environment dependent interaction potential (EDIP). The value of $\mathbf{E_d}$ in pristine graphite is found to be 20 eV, in agreement with previous molecular dynamics based calculations[5] and modern ab-initio density functional theory calculations in graphene[6]. It is found that $\mathbf{E_d}$ decreases for increasing irradiation damage, down to 5 eV at a irradiation dose of one displacement per atom. Probabilityof defect formation is classified according to the local environment of the primary knock-on atom and relationships between $\mathbf{E_d}$ and graphitic structure and texture are established.

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