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Threshold Displacement Energies of Oxygen in YBa2Cu3O7: A Multi-Physics Analysis

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High-temperature superconductors (HTS) are promising materials for next-generation fusion reactors and particle accelerators, owing to their remarkable field strengths at elevated temperatures. In these environments, radiation will impinge on the HTS, causing damage. Assessing the extent and nature of this damage is essential for determining the material's lifespan and any necessary shielding requirements.

The threshold displacement energy (TDE) can be used in predictive radiation damage models to predict material damage under radiation fluence. We provide the tools to assess the radiation hardness of YBa2Cu3O7 (YBCO) HTS by calculation of the TDE for all symmetrically distinct oxygen atoms. These results are obtained using an existing empirical potential, which we subsequently validate by a large-scale DFT investigation of TDEs in YBCO. An averaged TDE for the O atoms in YBCO is provided for use in analytical damage models, at temperatures of 25 and 360 K. Compared to previous work, we find decreased TDEs, and propose a number of defect structures that, to the best of our knowledge, have not yet been reported for YBCO.

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