Defect creation by radiation damage in $YBa_2Cu_3O_7$ high temperature superconductors

A. Dickson*[1], M. Gilbert[2], D. Nguyen-Manh[2], and S. T. Murphy*[1]

[1]School of Engineering, Lancaster University, Bailrigg, Lancaster LA1 4YW

[2]United Kingdom Atomic Energy Authority, Culham Campus, Abingdon, Oxon, OX14 3DB, UK

* Contact: a.dickson2@lancaster.ac.uk, samuel.murphy@lancaster.ac.uk

High-temperature superconductors (HTS) are increasingly popular in the design of future fusion reactors, owing to their remarkable field strengths at relatively high temperatures. It is crucial to assess the viability of these materials under operational conditions, where high energy neutron irradiation threatens to damage the HTS. Understanding the extent of this damage is pivotal to estimating material lifespan and determining the requisite shielding within the reactor. However, experimental reproduction of 'fast' neutrons represents significant challenges.

Theoretical approaches to predicting defect creation due to irradiation are all based on the energy that is required to displace an atom from its site to form a defect, the so-called threshold displacement energy, T_d. While models such as that of Kinchin-Pease [1] assume a single value for the displacement energy, molecular dynamics (MD) simulations show that this quantity exhibits a complex dependency on the crystal structure surrounding the primary knock-on atom (pka). There have been previous attempts to determine T_d for oxygen in $YBa_2Cu_3O_7$ using classical MD, however, there is some concern over the reliability of the potential models for this material. Therefore, we use ab initio MD to calculate the T_d and explore the different types of defects that are created during very low energy cascades.

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